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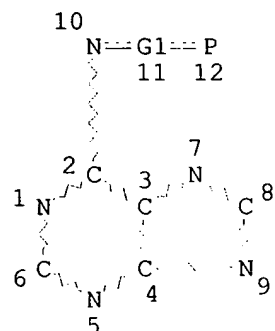
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FILE 'REGISTRY' ENTERED AT 13:28:43 ON 21 JUN 2002

L1 STR
L2 1 S L1
L3 144 S L1 FUL
L4 STR L1
L5 140 SEARCH L4 SUB=L3 FUL

=> d 15 que stat;d 1-140 ide cbib abs

L1 STR

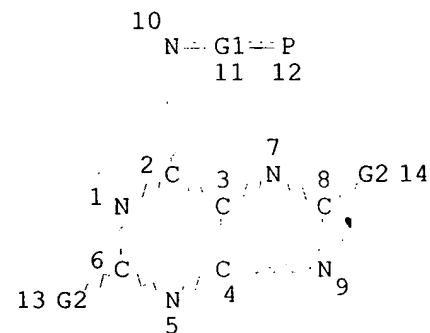


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NODE ATTRIBUTES:
CONNECT IS E2 RC AT 1
CONNECT IS E2 RC AT 5
CONNECT IS E2 RC AT 7
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE

L3 144 SEA FILE=REGISTRY SSS FUL L1
L4 STR



C @15

Searched by: Mary Hale 308-4258 CM-1 1E01

Burch
740653

09, 740, 653

REP G1=(0-20) A
VAR G2=H/X/O/S/N/15
NODE ATTRIBUTES:
NSPEC IS RC AT 15
CONNECT IS E2 RC AT 1
CONNECT IS E2 RC AT 5
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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE
L5 140 SEA FILE=REGISTRY SUB=L3 SSS FUL L4

100.0% PROCESSED 144 ITERATIONS 140 ANSWERS
SEARCH TIME: 00.00.02

L5 ANSWER 1 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 331473-84-8 REGISTRY
CN 3'-Cytidylic acid, 5'-O-phosphonocytidylyl-(3'.fwdarw.5')-,
3'-[19,39,59,65,85,105,108-heptahydroxy-63-(2-nitrophenyl)-
19,39,59,65,85,105-hexaoxido-115-oxo-120-(1H-purin-6-ylamino)-
3,6,9,12,15,18,20,23,26,29,32,35,38,40,43,46,49,52,55,58,60,64,66,69,72,75
,78,81,84,86,89,92,95,98,101,104,106,110-octatriacontaoxa-114-aza-
19,39,59,65,85,105-hexaphosphaeicosahect-1-yl] ester (9CI) (CA INDEX
NAME)
FS STEREOSEARCH
MF C104 H188 N13 O72 P9
SR CA
LC STN Files: CA, CAPLUS

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 134:252583 Multifunctional dinucleotide analogs for the
generation of complex RNA conjugates. Hausch, F.; Jaschke, A. (Institute
of Chemistry-Biochemistry, Free University Berlin, Berlin, D-14195,
Germany). Tetrahedron, 57(7), 1261-1268 (English) 2001. CODEN: TETRAB.
ISSN: 0040-4020. Publisher: Elsevier Science Ltd..

AB Oligonucleotide conjugates are needed for in vitro selection schemes
aiming at reactions between small, org. reactants. A general strategy is
provided for the generation of the required RNA reactant conjugates based
on multifunctional dinucleotide analogs. These modified dinucleotides
allow for enzymic ligation to native or enzymically transcribed RNAs.
They further contain a flexible polyethylene glycol spacer for correct
spatial positioning and a photolabile cleavage site for selective release.
The dinucleotides can be derivatized with the desired org. compds. by
activated ester chem. as was demonstrated by coupling to several
nucleobases and nucleotides.

L5 ANSWER 2 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 218146-51-1 REGISTRY
CN 3H-Indolium, 2-[5-[1-[3-[[[6-[9-[2-deoxy-5-O-
[hydroxy[hydroxy(phosphonooxy)phosphinyl]oxy]phosphinyl]-.beta.-D-erythro-

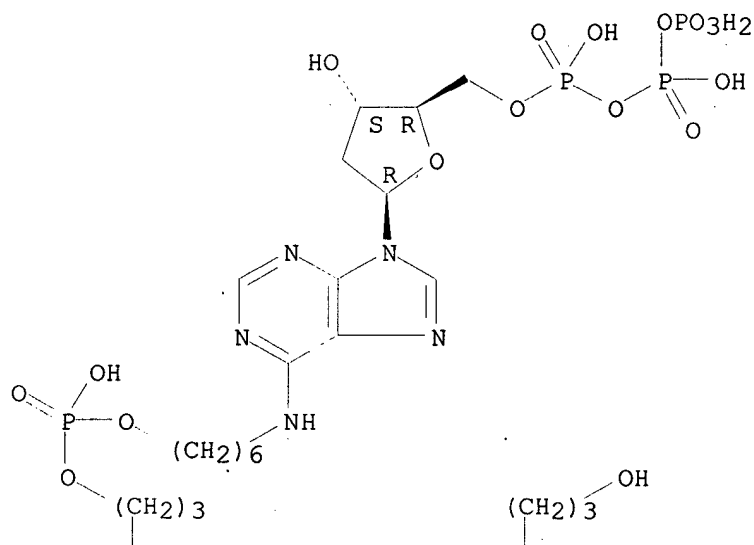
Searched by: Mary Hale 308-4258 CM-1 1E01

pentofuranosyl]-9H-purin-6-yl]amino]hexyl]oxy]hydroxyphosphinyl]oxy]propyl
]-1,3-dihydro-3,3-dimethyl-2H-indol-2-ylidene]-1,3-pentadienyl]-1-(3-
 hydroxypropyl)-3,3-dimethyl- (9CI) (CA INDEX NAME)

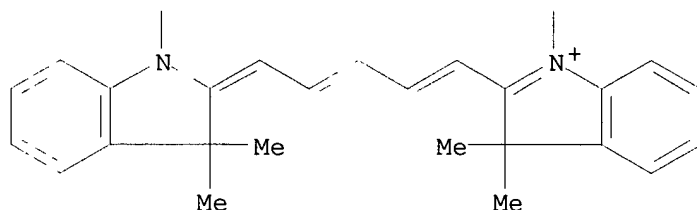
FS STEREOSEARCH
 MF C47 H66 N7 O17 P4
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.
 Double bond geometry unknown.

PAGE 1-A



PAGE 2-A

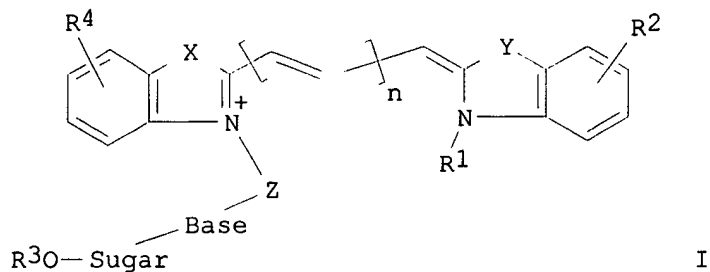


1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 130:66737 Preparation of non-sulfonated cyanine dyes for labeling nucleosides and nucleotides. Brush, Charles K.; Reimer, Ned D. (Amersham Pharmacia Biotech Inc., USA). PCT Int. Appl. WO 9858942 A1 19981230, 37 pp. DESIGNATED STATES: W: CA, JP; RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1998-US12593 19980616. PRIORITY: US 1997-879596 19970620.

Searched by: Mary Hale 308-4258 CM-1 1E01

GI



AB A chem. compd. of formula: I, wherein R1 is selected from the group consisting of alkyl, aralkyl, and substituted alkyl groups; R3 is selected from the group consisting of H, PO3-2; P2O6-3; P3O9-4, and .alpha.-thio phosphates (PSO2-2; P2SO5-3; P3SO8-4); and .alpha.BH3- phosphates (P(BH3)O2-2, P2(BH3)O5-3, P3(BH3)O8-4); R4 is selected from the group consisting of H, lower alkyl, acyl, (CH2)pCOO(CH2)qCH3 wherein p is an integer from 0 to 4 and q is an integer from 0 to 4, and 5,6; 6,7; or 7,8-butadienyl, R2 is selected from the group consisting of H, lower alkyl, acyl, (CH2)pCOO(CH2)qCH3 wherein p is an integer from 0 to 4 and q is an integer from 0 to 4 and 5,6; 6,7; or 7,8- butadienyl; n is 1, 2 or 3 to form a second fused arom.; X or Y are selected from the group consisting of O, S, C(R5)2, or N(R5), wherein R5 is preferably CH3 or a lower alkyl; and R3-O-Sugar-Base is a nucleoside or nucleotide is disclosed. Thus, 1-3''-(N4-6-amidohexyl-2',3'-dideoxycytidine-5'-O-triphosphate)-succinoyloxypropyl)-1'-(3'''-hydroxypropyl)-3,3,3',3'-tetramethylindodicarbocyanine was prepd. from N4-(6-aminoethyl)-ddCTP and indodicarbocyanine-NHS ester in 59 % yield.

L5 ANSWER 3 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 213541-77-6 REGISTRY

CN 5'-Adenylic acid, N-[13,33,39,59-tetrahydroxy-35-(2-nitrophenyl)-13,33,39,59-tetraoxido-8-oxo-77-[(5'-O-phosphonocytidylyl-(3'.fwdarw.5')-3'-cytidylyl)oxy]-12,14,17,20,23,26,29,32,34,38,40,43,46,49,52,55,58,60,63,66,69,72,75-tricosaoxa-7-aza-13,33,39,59-tetraphosphaheptaheptacont-1-yl]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

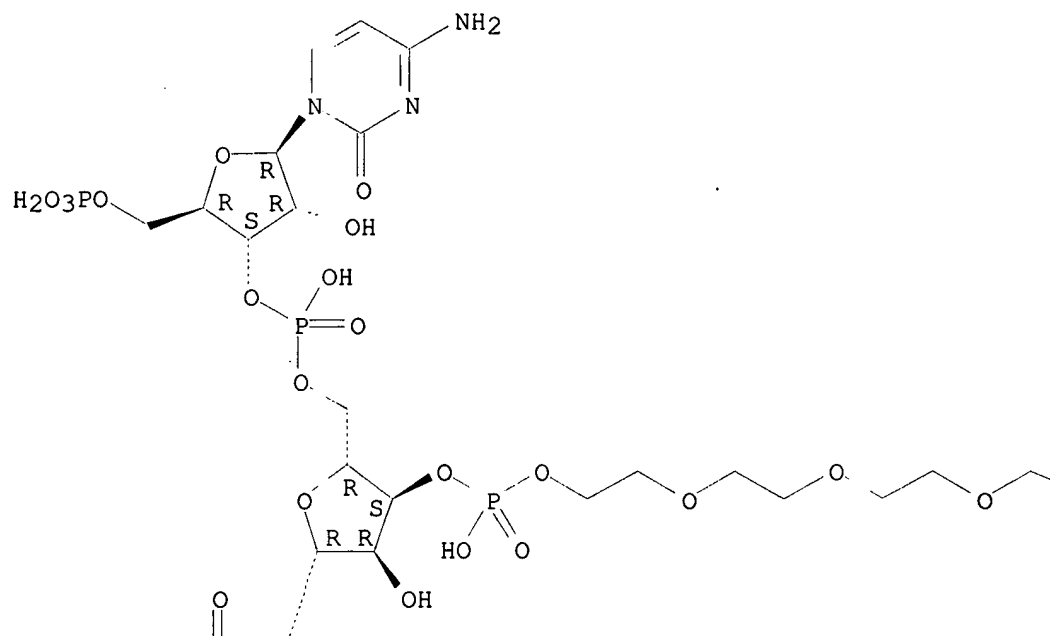
MF C83 H143 N13 O59 P8

SR CA

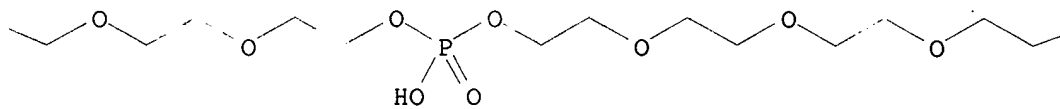
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

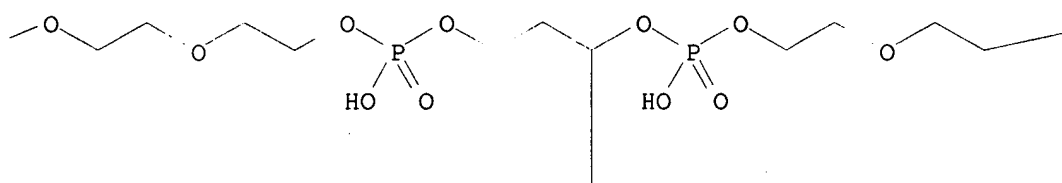
PAGE 1-A



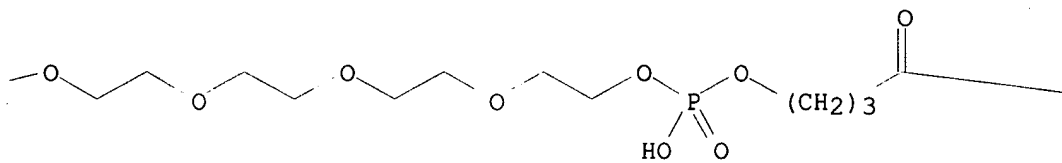
PAGE 1-B



PAGE 1-C



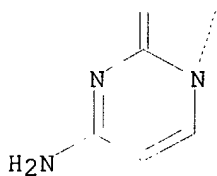
PAGE 1-D



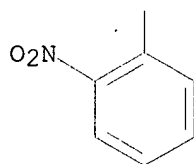
PAGE 1-E

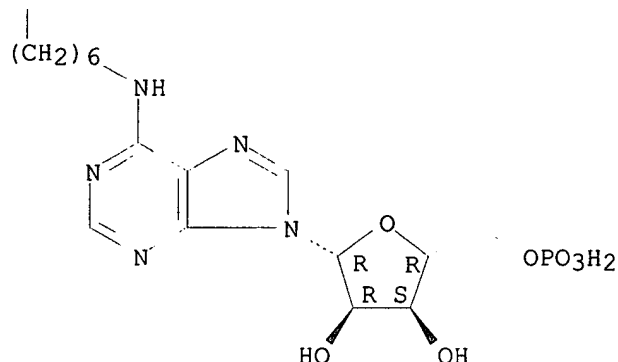


PAGE 2-A



PAGE 2-C





PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 134:252583 Multifunctional dinucleotide analogs for the generation of complex RNA conjugates. Hausch, F.; Jaschke, A. (Institute of Chemistry-Biochemistry, Free University Berlin, Berlin, D-14195, Germany). Tetrahedron, 57(7), 1261-1268 (English) 2001. CODEN: TETRAB. ISSN: 0040-4020. Publisher: Elsevier Science Ltd..

AB Oligonucleotide conjugates are needed for in vitro selection schemes aiming at reactions between small, org. reactants. A general strategy is provided for the generation of the required RNA reactant conjugates based on multifunctional dinucleotide analogs. These modified dinucleotides allow for enzymic ligation to native or enzymically transcribed RNAs. They further contain a flexible polyethylene glycol spacer for correct spatial positioning and a photolabile cleavage site for selective release. The dinucleotides can be derivatized with the desired org. compds. by activated ester chem. as was demonstrated by coupling to several nucleobases and nucleotides.

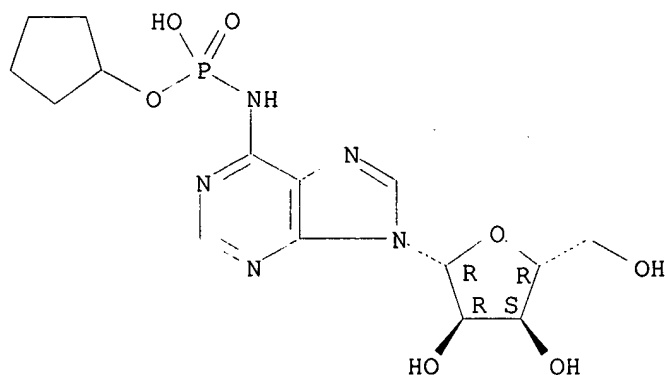
REFERENCE 2: 129:260732 A novel carboxy-functionalized photo-cleavable dinucleotide analog for the selection of RNA catalysts. Hausch, Felix; Jaschke, Andres (Institut fur Biochemie, Freie Universitat Berlin, Berlin, D-14195, Germany). Tetrahedron Letters, 39(34), 6157-6158 (English) 1998. CODEN: TELEAY. ISSN: 0040-4039. Publisher: Elsevier Science Ltd..

AB A new multifunctional dinucleotide analog is synthesized for the application in in vitro selection expts. with linker-coupled reactants. For this purpose it contains a 5'-pCC ligation site, three flexible-hexaethylene glycol spacers, a photo-cleavable o-nitrobenzyl unit and a 3'-terminal carboxy-function which can be derivatized with potential reactants as demonstrated with three model compds.

L5 ANSWER 4 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 199182-37-1 REGISTRY
CN Adenosine, N-[(cyclopentyloxy)hydroxyphosphinyl]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C15 H22 N5 O7 P
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Searched by: Mary Hale 308-4258 CM-1 1E01



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 128:13393 A study towards total synthesis of antibiotic Agrocine 84. Filippov, Dmitri; Timmers, Cornelis M.; van der Marel, Gijs A.; van Boom, Jacques H. (Gorlaeus Laboratories, Leiden Institute of Chemistry, Leiden, 2300 RA, Neth.). Nucleosides & Nucleotides, 16(7-9), 1403-1406 (English) 1997. CODEN: NUNUD5. ISSN: 0732-8311. Publisher: Marcel Dekker, Inc..

AB A versatile synthetic route to an analog of the naturally occurring bacteriocin Agrocine 84 is described.

L5 ANSWER 5 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 199182-36-0 REGISTRY

CN Adenosine, N-[(cyclopentyloxy)hydroxyphosphinyl]-2',3'-bis-O-[(1,1-dimethylethyl)dimethylsilyl]-, 5'-[hydrogen [(2S)-2,3-bis[(1,1-dimethylethyl)dimethylsilyl]oxy]-1-oxopropyl]phosphoramidate] (9CI) (CA INDEX NAME)

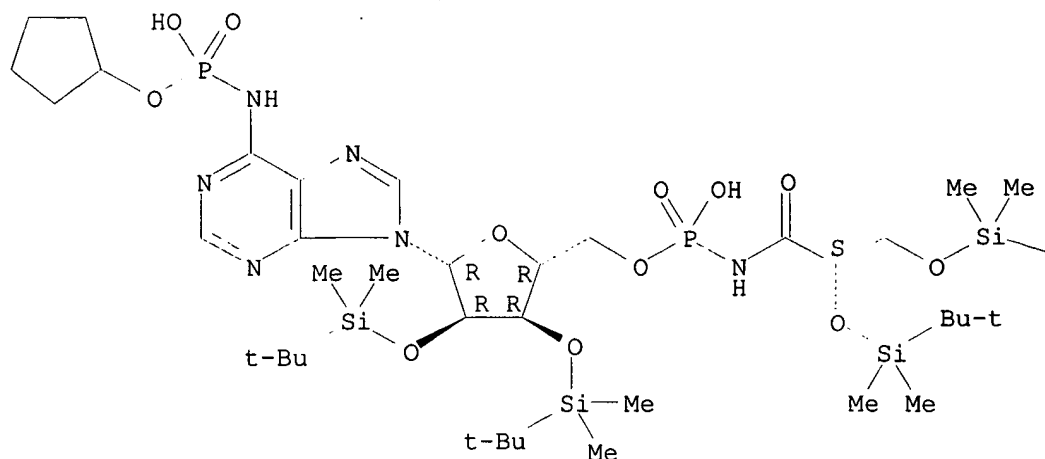
FS STEREOSEARCH

MF C42 H84 N6 O12 P2 Si4

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.



— Bu-t

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 128:13393 A study towards total synthesis of antibiotic Agrocine 84. Filippov, Dmitri; Timmers, Cornelis M.; van der Marel, Gijs A.; van Boom, Jacques H. (Gorlaeus Laboratories, Leiden Institute of Chemistry, Leiden, 2300 RA, Neth.). Nucleosides & Nucleotides, 16(7-9), 1403-1406 (English) 1997. CODEN: NUNUD5. ISSN: 0732-8311. Publisher: Marcel Dekker, Inc..

AB A versatile synthetic route to an analog of the naturally occurring bacteriocin Agrocine 84 is described.

L5 ANSWER 6 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 199182-32-6 REGISTRY

CN Adenosine, N-[(2-cyanoethoxy)(cyclopentylthio)phosphinyl]-2',3'-bis-O-[(1,1-dimethylethyl)dimethylsilyl]-, 5'-[2-cyanoethyl {(2S)-2,3-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-1-oxopropyl}phosphoramidate] (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C48 H90 N8 O12 P2 Si4

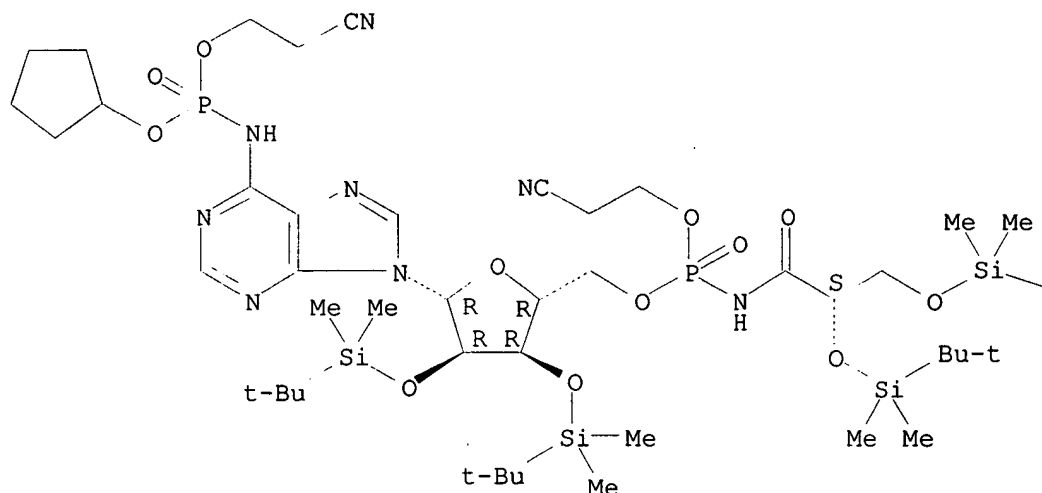
SR CA

LC STN Files: CA, CAPLUS

Searched by: Mary Hale 308-4258 CM-1 1E01

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

Bu-t

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 128:13393 A study towards total synthesis of antibiotic Agrocine 84. Filippov, Dmitri; Timmers, Cornelis M.; van der Marel, Gijs A.; van Boom, Jacques H. (Gorlaeus Laboratories, Leiden Institute of Chemistry, Leiden, 2300 RA, Neth.). Nucleosides & Nucleotides, 16(7-9), 1403-1406 (English) 1997. CODEN: NUNUD5. ISSN: 0732-8311. Publisher: Marcel Dekker, Inc..

AB A versatile synthetic route to an analog of the naturally occurring bacteriocin Agrocine 84 is described.

L5 ANSWER 7 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 199182-31-5 REGISTRY

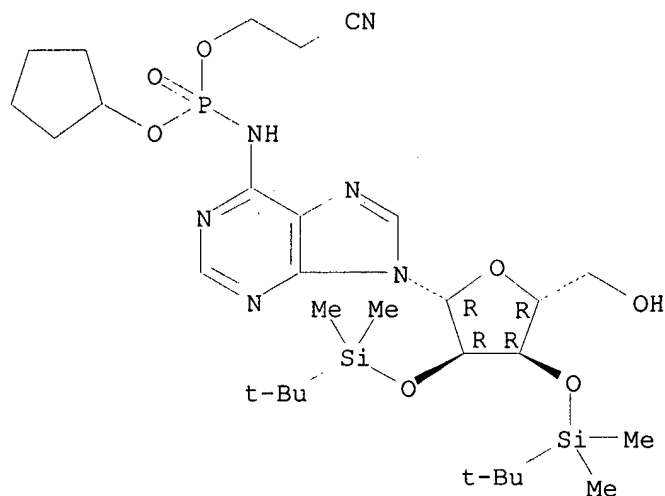
CN Adenosine, N-[(2-cyanoethoxy)(cyclopentylloxy)phosphinyl]-2',3'-bis-O-[(1,1-dimethylethyl)dimethylsilyl]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

Searched by: Mary Hale 308-4258 CM-1 1E01

MF C30 H53 N6 O7 P Si2
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 128:13393 A study towards total synthesis of antibiotic Agrocin 84. Filippov, Dmitri; Timmers, Cornelis M.; van der Marel, Gijs A.; van Boom, Jacques H. (Gorlaeus Laboratories, Leiden Institute of Chemistry, Leiden, 2300 RA, Neth.). Nucleosides & Nucleotides, 16(7-9), 1403-1406 (English) 1997. CODEN: NUNUD5. ISSN: 0732-8311. Publisher: Marcel Dekker, Inc..

AB A versatile synthetic route to an analog of the naturally occurring bacteriocin Agrocin 84 is described.

L5 ANSWER 8 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 199182-30-4 REGISTRY

CN Adenosine, 5'-O-[bis(4-methoxyphenyl)phenylmethyl]-N-[(2-cyanoethoxy)(cyclopentyloxy)phosphinyl]-2',3'-bis-O-[(1,1-dimethylethyl)dimethylsilyl]- (9CI) (CA INDEX NAME)

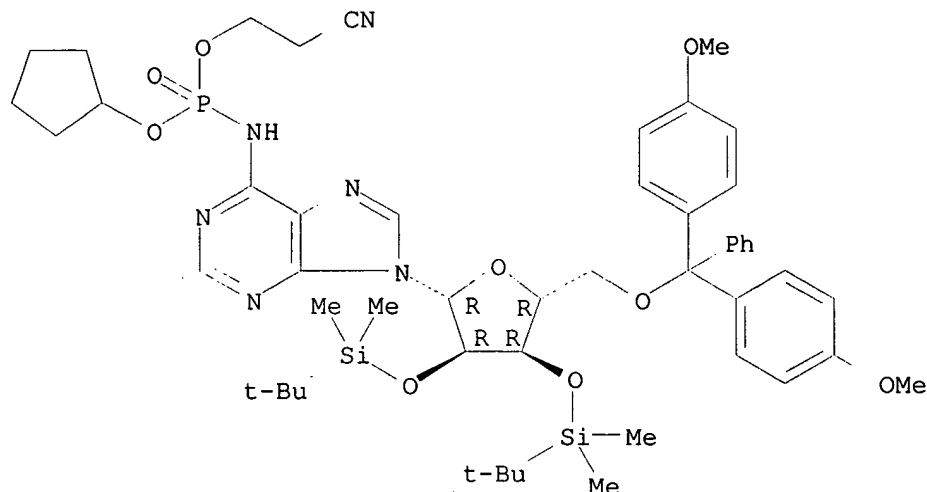
FS STEREOSEARCH

MF C51 H71 N6 O9 P Si2

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 128:13393 A study towards total synthesis of antibiotic Agrocine 84. Filippov, Dmitri; Timmers, Cornelis M.; van der Marel, Gijs A.; van Boom, Jacques H. (Gorlaeus Laboratories, Leiden Institute of Chemistry, Leiden, 2300 RA, Neth.). Nucleosides & Nucleotides, 16(7-9), 1403-1406 (English) 1997. CODEN: NUNUD5. ISSN: 0732-8311. Publisher: Marcel Dekker, Inc..

AB A versatile synthetic route to an analog of the naturally occurring bacteriocin Agrocine 84 is described.

L5 ANSWER 9 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 199182-27-9 REGISTRY

CN Adenosine, N-[(cyclopentyloxy)hydroxyphosphinyl]-, 5'-[hydrogen [(2S)-2,3-dihydroxy-1-oxopropyl]phosphoramidate] (9CI) (CA INDEX NAME)

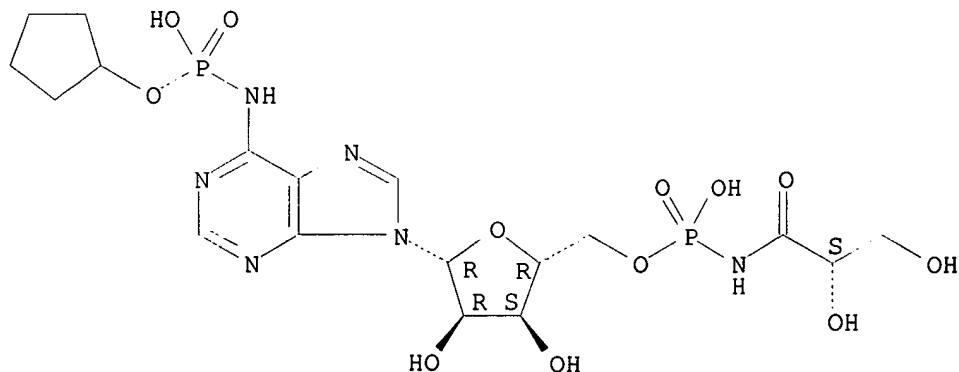
FS STEREOSEARCH

MF C18 H28 N6 O12 P2

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.



Searched by: Mary Hale 308-4258 CM-1 1E01

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 128:13393 A study towards total synthesis of antibiotic Agrocin 84. Filippov, Dmitri; Timmers, Cornelis M.; van der Marel, Gijs A.; van Boom, Jacques H. (Gorlaeus Laboratories, Leiden Institute of Chemistry, Leiden, 2300 RA, Neth.). Nucleosides & Nucleotides, 16(7-9), 1403-1406 (English) 1997. CODEN: NUNUD5. ISSN: 0732-8311. Publisher: Marcel Dekker, Inc..

AB A versatile synthetic route to an analog of the naturally occurring bacteriocin Agrocin 84 is described.

L5 ANSWER 10 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 184640-94-6 REGISTRY

CN Adenosine, N-(ethoxyhydroxyphosphinyl)-, monosodium salt (9CI) (CA INDEX NAME)

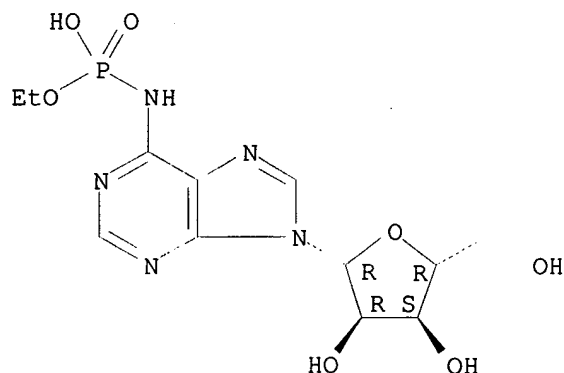
FS STEREOSEARCH

MF C12 H18 N5 O7 P . Na

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.



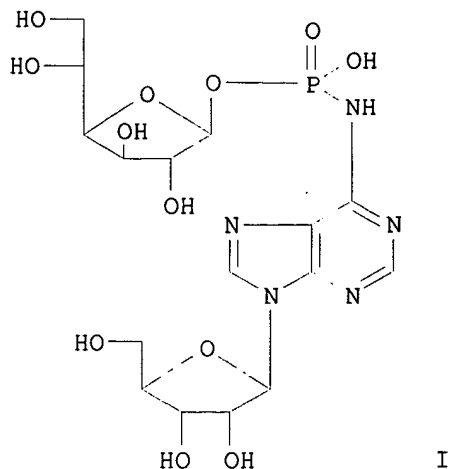
● Na

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:47468 New Nucleoside-Sugar Conjugates: 6-N-Glycosyloxyphosphorylated Adenosine Derivatives as Partial Structures of Agrocin 84. Moriguchi, Tomohisa; Wada, Takeshi; Sekine, Mitsuo (Department of Life Science, Tokyo Institute of Technology, Yokohama, 226, Japan). Journal of Organic Chemistry, 61(26), 9223-9228 (English) 1996. CODEN: JOCEAH. ISSN: 0022-3263. Publisher: American Chemical Society.

GI

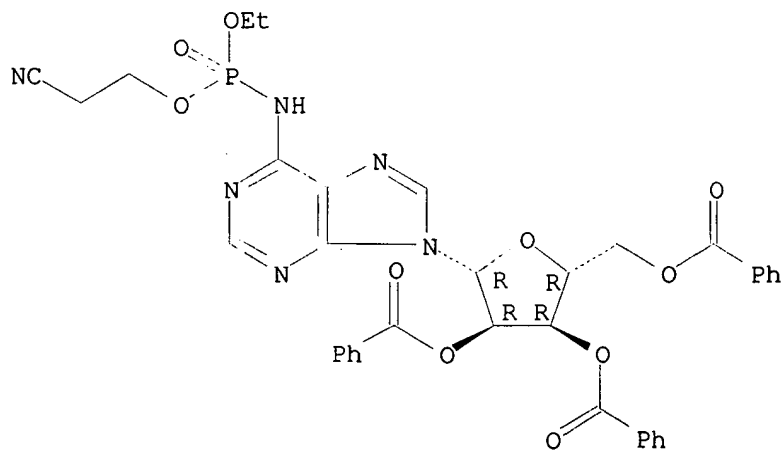
Searched by: Mary Hale 308-4258 CM-1 1E01



AB We report the first successful prepn. of glucofuranosyloxyphosphoryl adenosine I as a partial structure of agrocin 84 via a two-step phosphorylation of 2',3',5'-tri-O-benzoyladenosine with a 2,3,5,6-tetra-O-acetylglucofuranoside 1-O-phosphoramidite deriv. that has a 2-(trimethylsilyl)ethyl group as the phosphate protecting group. The stabilities of these 6-N-[(glycos-1-yloxy)phosphoryl]adenosine derivs. under acidic, basic, and thermal conditions are described. In particular, we found that the O-P bond of these sugar-nucleoside conjugates was selectively cleaved by treatment with 0.1 M NaOH to give 6-N-phosphoryladenosine, while acidic treatment gave directly adenosine with cleavage of the P-N bond.

L5 ANSWER 11 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 184640-93-5 REGISTRY
 CN Adenosine, N-[(2-cyanoethoxy)ethoxyphosphinyl]-, 2',3',5'-tribenzoate (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C36 H33 N6 O10 P
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.

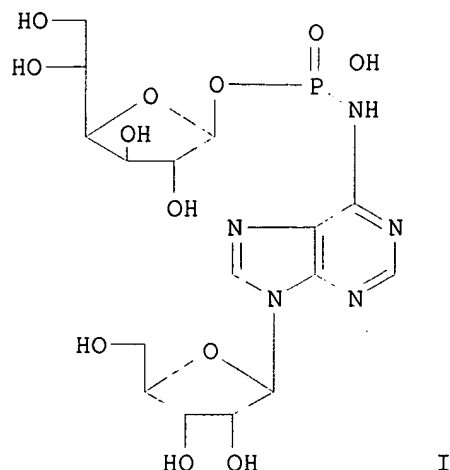


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:47468 New Nucleoside-Sugar Conjugates: 6-N-Glycosyloxyphosphorylated Adenosine Derivatives as Partial Structures of Agrocin 84. Moriguchi, Tomohisa; Wada, Takeshi; Sekine, Mitsuo (Department of Life Science, Tokyo Institute of Technology, Yokohama, 226, Japan). Journal of Organic Chemistry, 61(26), 9223-9228 (English) 1996. CODEN: JOCEAH. ISSN: 0022-3263. Publisher: American Chemical Society.

GI



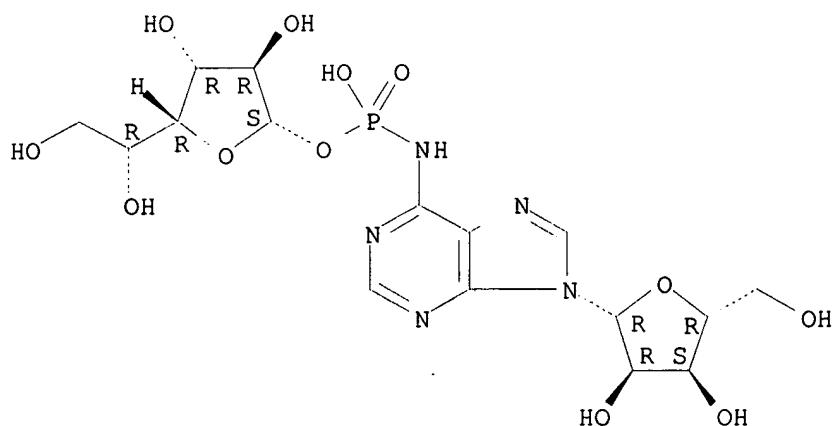
I

AB We report the first successful prepn. of glucofuranosyloxyphosphoryl adenosine I as a partial structure of agrocin 84 via a two-step phosphorylation of 2',3',5'-tri-O-benzoyl adenosine with a 2,3,5,6-tetra-O-acetylglucofuranoside 1-O-phosphoramidite deriv. that has a 2-(trimethylsilyl)ethyl group as the phosphate protecting group. The stabilities of these 6-N-[(glycos-1-yloxy)phosphoryl]adenosine derivs. under acidic, basic, and thermal conditions are described. In particular, we found that the O-P bond of these sugar-nucleoside conjugates was selectively cleaved by treatment with 0.1 M NaOH to give 6-N-phosphoryl adenosine, while acidic treatment gave directly adenosine with cleavage of the P-N bond.

L5 ANSWER 12 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 184640-92-4 REGISTRY
CN Adenosine, N-[(.beta.-D-glucofuranosyloxy)hydroxyphosphinyl]-, monosodium salt (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C16 H24 N5 O12 P . Na
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Searched by: Mary Hale 308-4258 CM-1 1E01

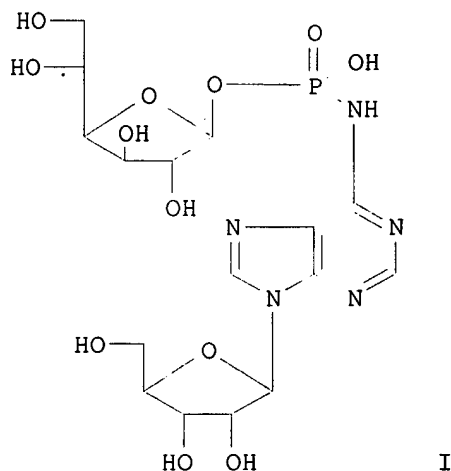


● Na

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:47468 New Nucleoside-Sugar Conjugates: 6-N-Glycosyloxyphosphorylated Adenosine Derivatives as Partial Structures of Agrocin 84. Moriguchi, Tomohisa; Wada, Takeshi; Sekine, Mitsuo (Department of Life Science, Tokyo Institute of Technology, Yokohama, 226, Japan). Journal of Organic Chemistry, 61(26), 9223-9228 (English) 1996. CODEN: JOCEAH. ISSN: 0022-3263. Publisher: American Chemical Society.

GI



I

AB We report the first successful prepn. of glucofuranosyloxyphosphoryl adenosine I as a partial structure of agrocin 84 via a two-step phosphorylation of 2',3',5'-tri-O-benzoyladenosine with a 2,3,5,6-tetra-O-acetylglucofuranoside 1-O-phosphoramidite deriv. that has a 2-(trimethylsilyl)ethyl group as the phosphate protecting group. The stabilities of these 6-N-[(glycos-1-yloxy)phosphoryl]adenosine derivs. under acidic, basic, and thermal conditions are described. In particular, we found that the O-P bond of these sugar-nucleoside conjugates was selectively cleaved by treatment with 0.1 M NaOH to give

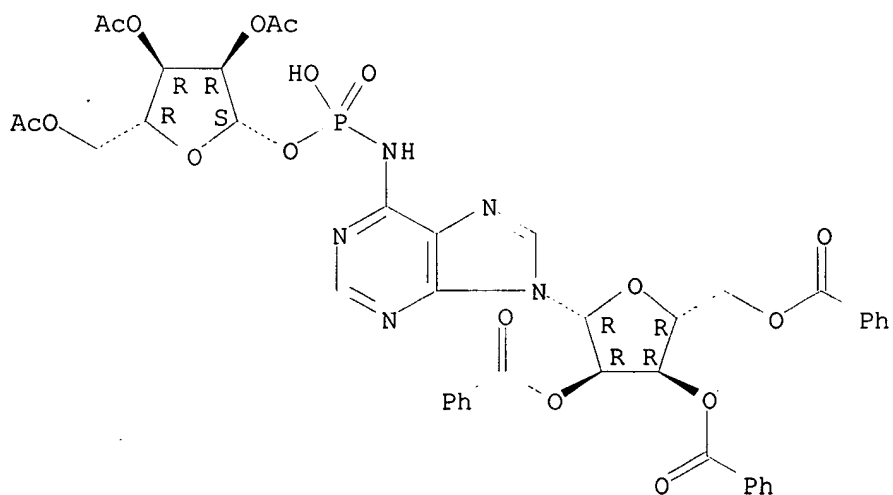
6-N-phosphoryladenossine, while acidic treatment gave directly adenosine with cleavage of the P-N bond.

L5 ANSWER 13 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 184640-89-9 REGISTRY
CN Adenosine, N-[hydroxy[(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)oxy]phosphinyl]-, 2',3',5'-tribenzoate, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C42 H40 N5 O17 P . C6 H15 N
SR CA
LC STN Files: CA, CAPLUS

CM 1

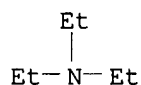
CRN 184640-88-8
CMF C42 H40 N5 O17 P

Absolute stereochemistry.



CM 2

CRN 121-44-8
CMF C6 H15 N

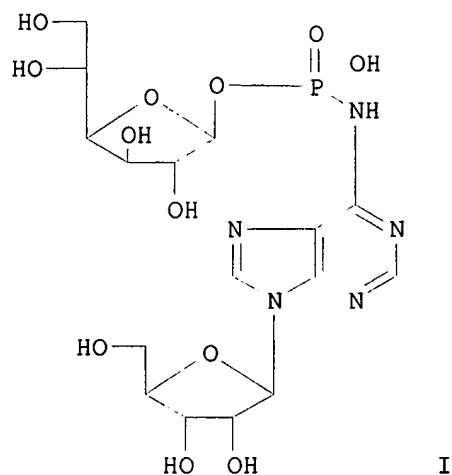


1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:47468 New Nucleoside-Sugar Conjugates: 6-N-Glycosyloxyphosphorylated Adenosine Derivatives as Partial Structures of Agrocine 84. Moriguchi, Tomohisa; Wada, Takeshi; Sekine, Mitsuo (Department of Life Science, Tokyo Institute of Technology, Yokohama, 226, Japan). Journal of Organic Chemistry, 61(26), 9223-9228 (English) 1996. CODEN: JOCEAH. ISSN: 0022-3263. Publisher: American Chemical Society.

GI

Searched by: Mary Hale 308-4258 CM-1 1E01



AB We report the first successful prepn. of glucofuranosyloxyphosphoryl adenosine I as a partial structure of agrocin 84 via a two-step phosphorylation of 2',3',5'-tri-O-benzoyladenosine with a 2,3,5,6-tetra-O-acetylglucofuranoside 1-O-phosphoramidite deriv. that has a 2-(trimethylsilyl)ethyl group as the phosphate protecting group. The stabilities of these 6-N-[(glycos-1-yloxy)phosphoryl]adenosine derivs. under acidic, basic, and thermal conditions are described. In particular, we found that the O-P bond of these sugar-nucleoside conjugates was selectively cleaved by treatment with 0.1 M NaOH to give 6-N-phosphoryladenosine, while acidic treatment gave directly adenosine with cleavage of the P-N bond.

L5 ANSWER 14 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 184640-88-8 REGISTRY

CN Adenosine, N-[hydroxy[(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)oxy]phosphinyl]-, 2',3',5'-tribenzoate (9CI) (CA INDEX NAME)

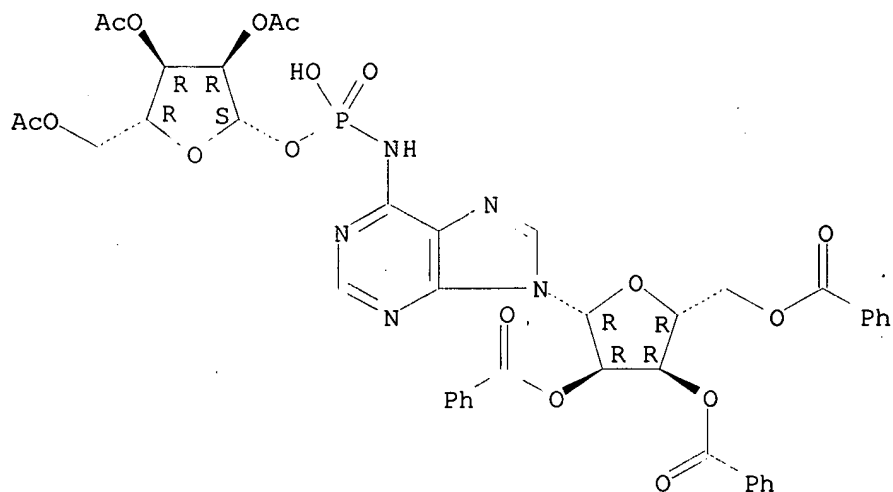
FS STEREOSEARCH

MF C42 H40 N5 O17 P

CI COM

SR CA

Absolute stereochemistry.



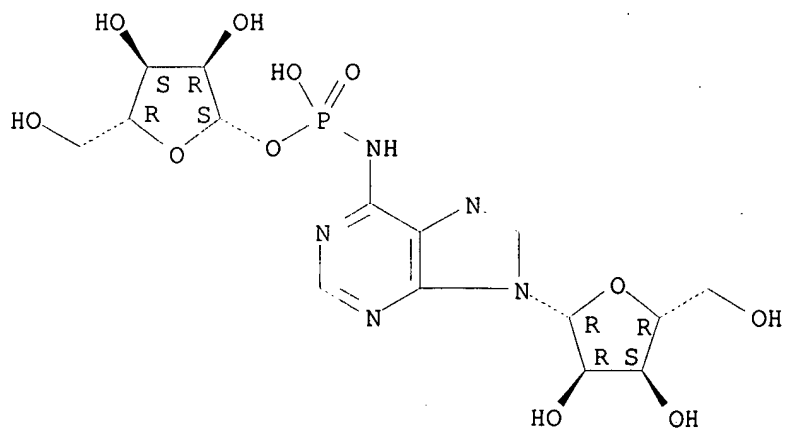
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 15 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 184640-87-7 REGISTRY
 CN Adenosine, N-[hydroxy(.beta.-D-ribofuranosyloxy)phosphinyl]-, compd. with
 N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C15 H22 N5 O11 P . C6 H15 N
 SR CA
 LC STN Files: CA, CAPLUS

CM 1

CRN 184640-86-6
 CMF C15 H22 N5 O11 P

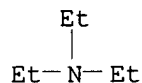
Absolute stereochemistry.



CM 2

CRN 121-44-8
 CMF C6 H15 N

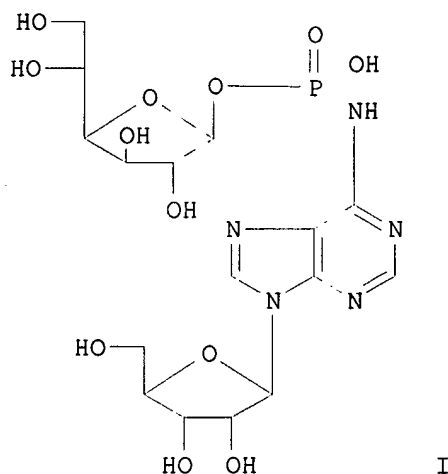
Searched by: Mary Hale 308-4258 CM-1 1E01



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 126:47468 New Nucleoside-Sugar Conjugates: 6-N-Glycosyloxyphosphorylated Adenosine Derivatives as Partial Structures of Agrocine 84. Moriguchi, Tomohisa; Wada, Takeshi; Sekine, Mitsuo (Department of Life Science, Tokyo Institute of Technology, Yokohama, 226, Japan). Journal of Organic Chemistry, 61(26), 9223-9228 (English) 1996. CODEN: JOCEAH. ISSN: 0022-3263. Publisher: American Chemical Society.

GI

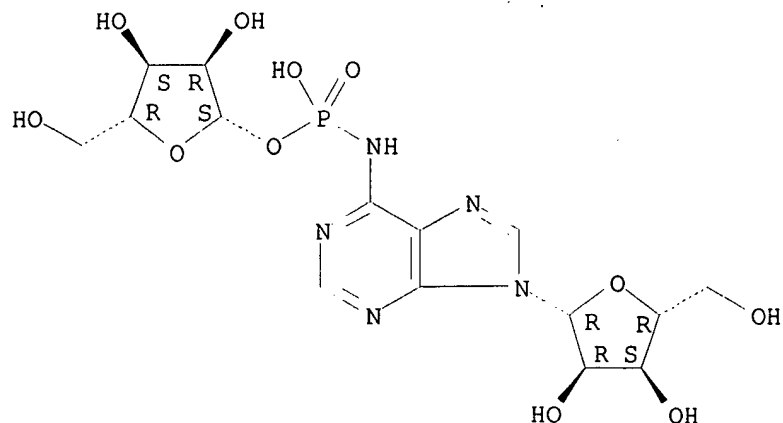


AB We report the first successful prepn. of glucofuranosyloxyphosphoryl adenosine I as a partial structure of agrocine 84 via a two-step phosphorylation of 2',3',5'-tri-O-benzoyladenosine with a 2,3,5,6-tetra-O-acetylglucosylphosphoramide deriv. that has a 2-(trimethylsilyl)ethyl group as the phosphate protecting group. The stabilities of these 6-N-[(glycosyl-yloxy)phosphoryl]adenosine derivs. under acidic, basic, and thermal conditions are described. In particular, we found that the O-P bond of these sugar-nucleoside conjugates was selectively cleaved by treatment with 0.1 M NaOH to give 6-N-phosphoryladenosine, while acidic treatment gave directly adenosine with cleavage of the P-N bond.

L5 ANSWER 16 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 184640-86-6 REGISTRY
CN Adenosine, N-[hydroxy(.beta.-D-ribofuranosyloxy)phosphinyl]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C15 H22 N5 O11 P
CI COM
SR CA

Searched by: Mary Hale 308-4258 CM-1 1E01

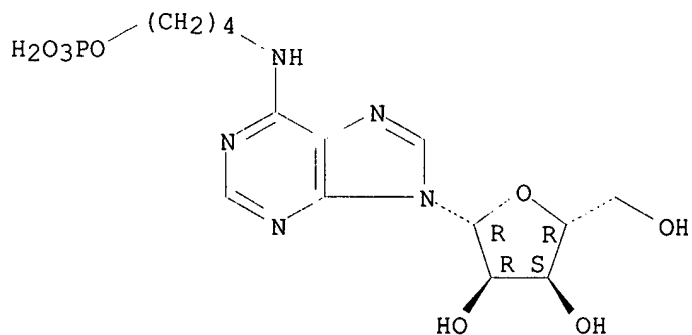
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 17 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 182950-56-7 REGISTRY
CN Adenosine, N-[4-(phosphonooxy)butyl]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C14 H22 N5 O8 P
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



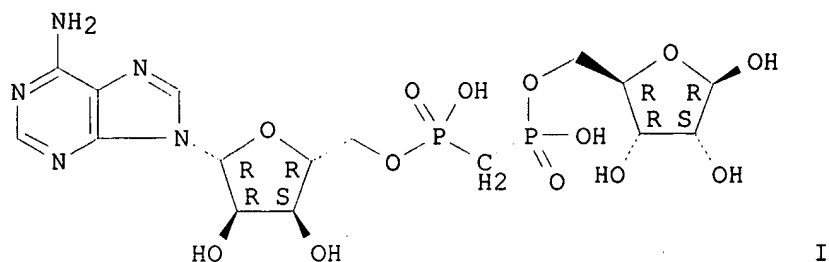
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 125:301465 Synthesis of methylenebis(phosphonate) analogs of ADP-Ribose. Pankiewicz, Krzysztof W.; Lesiak, Krystyna; Zatorski, Andrzej; Watanabe, Kyoichi A. (OncorPharm, Inc., Gaithersburg, MD, 20877, USA). Collect. Czech. Chem. Commun., 61(Spec. Issue), S92-S95 (English) 1996. CODEN: CCCCAK. ISSN: 0010-0765.

GI

Searched by: Mary Hale 308-4258 CM-1 1E01



AB An efficient synthesis of analogs of ADP-ribose contg. a methylene group instead of pyrophosphate oxygen is described. A target compd. was the ribose analog I. Formation of a cADP-ribose analog and cIDP-ribose analogs, in which N1-ribose was replaced by butanol, was also reported.

L5 ANSWER 18 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 167780-59-8 REGISTRY

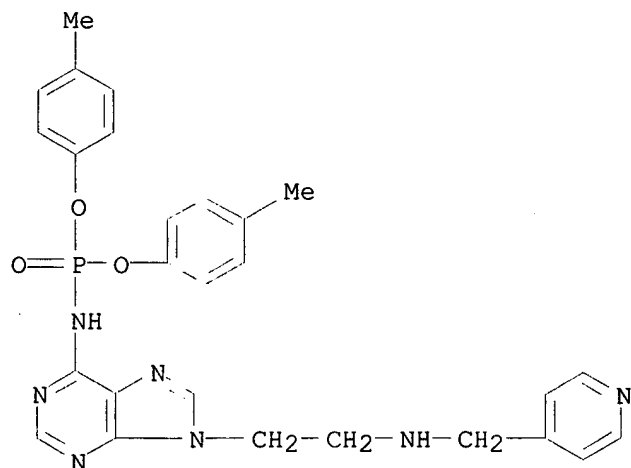
CN Phosphoramidic acid, [9-[2-[(4-pyridinylmethyl)amino]ethyl]-9H-purin-6-yl]-, bis(4-methylphenyl) ester (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C27 H28 N7 O3 P

SR CA

LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

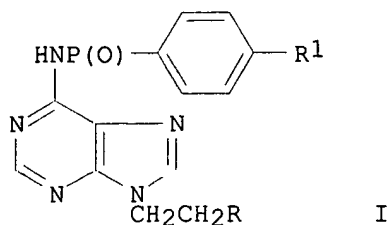
1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:198508 Phosphorylated adenine derivatives as potential synthons for antiviral agents. El Masri, Marwan; Berlin, K. Darrell (Dep. Chem., Oklahoma State Univ., Stillwater, OK, 74078, USA). Org. Prep. Proced. Int., 27(2), 161-9 (English) 1995. CODEN: OPPIAK. ISSN: 0030-4948.

GI

Searched by: Mary Hale 308-4258 CM-1 1E01



AB Phosphorylated adenines I [R = Cl; R1 = H, Me] were prepd. from 9-(2-hydroxyethyl)adenine (II) by reaction with ClP(O)(OC6H4R1-4)2. I [R = Cl] were converted to I [R = N3, pyridylamino]. II was also converted to phosphate esters and phosphonates and phosphates of aniline and 4-aminopyridine were also prepd.

L5 ANSWER 19 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 167780-58-7 REGISTRY

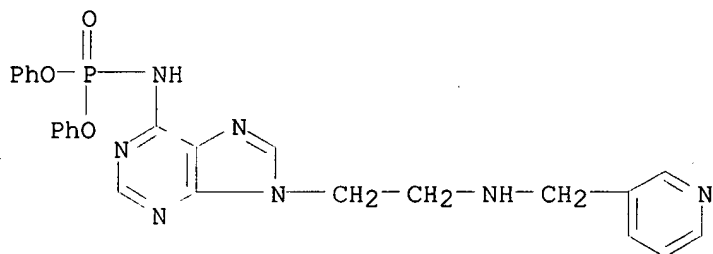
CN Phosphoramidic acid, [9-[2-[(3-pyridinylmethyl)amino]ethyl]-9H-purin-6-yl]-, diphenyl ester (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C25 H24 N7 O3 P

SR CA

LC STN Files: CA, CAPLUS



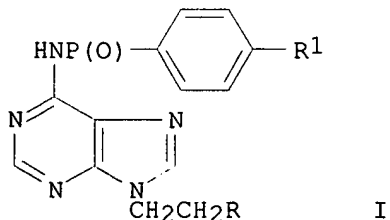
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:198508 Phosphorylated adenine derivatives as potential synthons for antiviral agents. El Masri, Marwan; Berlin, K. Darrell (Dep. Chem., Oklahoma State Univ., Stillwater, OK, 74078, USA). Org. Prep. Proced. Int., 27(2), 161-9 (English) 1995. CODEN: OPPIAK. ISSN: 0030-4948.

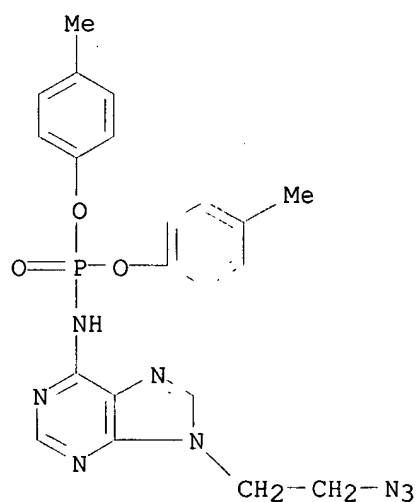
GI



Searched by: Mary Hale 308-4258 CM-1 1E01

AB Phosphorylated adenines I [R = Cl; R1 = H, Me] were prepd. from 9-(2-hydroxyethyl)adenine (II) by reaction with ClP(O)(OC6H4R1-4)2. I [R = Cl] were converted to I [R = N3, pyridylamino]. II was also converted to phosphate esters and phosphonates and phosphates of aniline and 4-aminopyridine were also prepd.

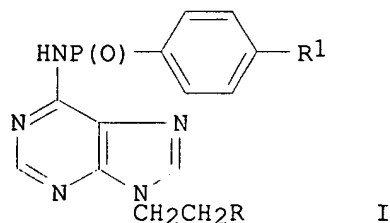
L5 ANSWER 20 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 167780-57-6 REGISTRY
 CN Phosphoramidic acid, [9-(2-azidoethyl)-9H-purin-6-yl]-, bis(4-methylphenyl) ester (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C21 H21 N8 O3 P
 SR CA
 LC STN Files: CA, CAPLUS



1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:198508 Phosphorylated adenine derivatives as potential synthons for antiviral agents. El Masri, Marwan; Berlin, K. Darrell (Dep. Chem., Oklahoma State Univ., Stillwater, OK, 74078, USA). Org. Prep. Proced. Int., 27(2), 161-9 (English) 1995. CODEN: OPPIAK. ISSN: 0030-4948.

GI

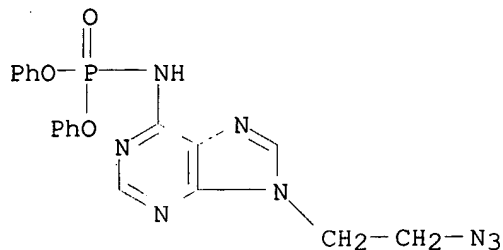


AB Phosphorylated adenines I [R = Cl; R1 = H, Me] were prepd. from 9-(2-hydroxyethyl)adenine (II) by reaction with ClP(O)(OC6H4R1-4)2. I [R

Searched by: Mary Hale 308-4258 CM-1 1E01

= Cl] were converted to I [R = N3, pyridylamino]. II was also converted to phosphate esters and phosphonates and phosphates of aniline and 4-aminopyridine were also prepd.

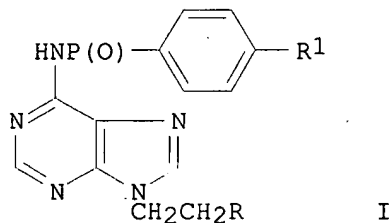
L5 ANSWER 21 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 167780-56-5 REGISTRY
 CN Phosphoramidic acid, [9-(2-azidoethyl)-9H-purin-6-yl]-, diphenyl ester (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C19 H17 N8 O3 P
 SR CA
 LC STN Files: CA, CAPLUS



1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:198508 Phosphorylated adenine derivatives as potential synthons for antiviral agents. El Masri, Marwan; Berlin, K. Darrell (Dep. Chem., Oklahoma State Univ., Stillwater, OK, 74078, USA). Org. Prep. Proced. Int., 27(2), 161-9 (English) 1995. CODEN: OPPIAK. ISSN: 0030-4948.

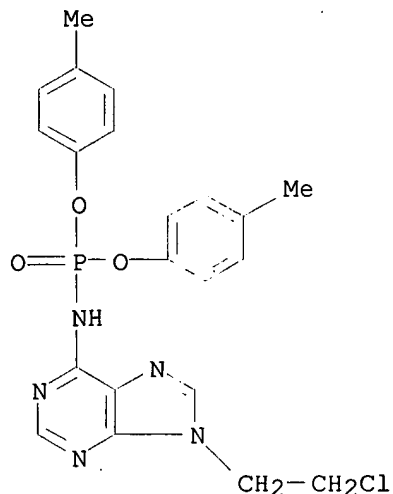
GI



AB Phosphorylated adenines I [R = Cl; R1 = H, Me] were prepd. from 9-(2-hydroxyethyl)adenine (II) by reaction with ClP(O)(OC6H4R1-4)2. I [R = Cl] were converted to I [R = N3, pyridylamino]. II was also converted to phosphate esters and phosphonates and phosphates of aniline and 4-aminopyridine were also prepd.

L5 ANSWER 22 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 167780-55-4 REGISTRY
 CN Phosphoramidic acid, [9-(2-chloroethyl)-9H-purin-6-yl]-, bis(4-methylphenyl) ester (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C21 H21 Cl N5 O3 P
 SR CA
 LC STN Files: CA, CAPLUS

Searched by: Mary Hale 308-4258 CM-1 1E01

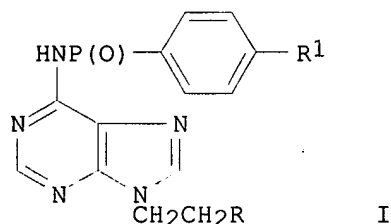


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:198508 Phosphorylated adenine derivatives as potential synthons for antiviral agents. El Masri, Marwan; Berlin, K. Darrell (Dep. Chem., Oklahoma State Univ., Stillwater, OK, 74078, USA). Org. Prep. Proced. Int., 27(2), 161-9 (English) 1995. CODEN: OPPIAK. ISSN: 0030-4948.

GI

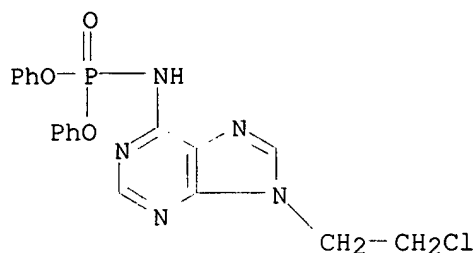


I

AB Phosphorylated adenines I [R = Cl; R1 = H, Me] were prepd. from 9-(2-hydroxyethyl)adenine (II) by reaction with ClP(O)(OC6H4R1-4)2. I [R = Cl] were converted to I [R = N3, pyridylamino]. II was also converted to phosphate esters and phosphonates and phosphates of aniline and 4-aminopyridine were also prepd.

L5 ANSWER 23 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 167780-54-3 REGISTRY
CN Phosphoramidic acid, [9-(2-chloroethyl)-9H-purin-6-yl]-, diphenyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H17 Cl N5 O3 P
SR CA
LC STN Files: CA, CAPLUS

Searched by: Mary Hale 308-4258 CM-1 1E01

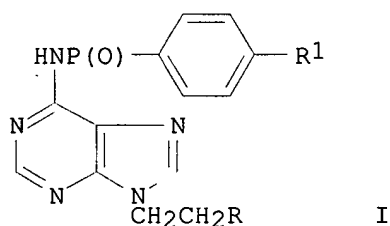


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:198508 Phosphorylated adenine derivatives as potential synthons for antiviral agents. El Masri, Marwan; Berlin, K. Darrell (Dep. Chem., Oklahoma State Univ., Stillwater, OK, 74078, USA). Org. Prep. Proced. Int., 27(2), 161-9 (English) 1995. CODEN: OPPIAK. ISSN: 0030-4948.

GI



AB Phosphorylated adenines I [R = Cl; R1 = H, Me] were prepd. from 9-(2-hydroxyethyl)adenine (II) by reaction with ClP(O)(OC6H4R1-4)2. I [R = Cl] were converted to I [R = N3, pyridylamino]. II was also converted to phosphate esters and phosphonates and phosphates of aniline and 4-aminopyridine were also prepd.

L5 ANSWER 24 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 161879-76-1 REGISTRY

CN Phosphoramidothioic acid, (9-.beta.-D-ribofuranosyl-9H-purin-6-yl)-, O,O-diethyl ester (9CI) (CA INDEX NAME)

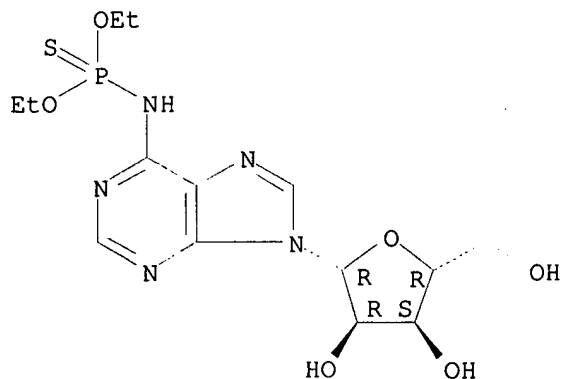
FS STEREOSEARCH

MF C14 H22 N5 O6 P S

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

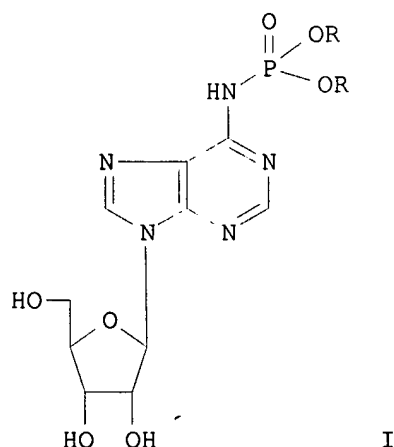


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 122:214406 Synthesis and Properties of N-Phosphorylated Ribonucleosides. Wada, Takeshi; Moriguchi, Tomohisa; Sekine, Mitsuo (Faculty of Bioscience and Biotechnology, Tokyo Institute of Technology, Yokohama, 227, Japan). J. Am. Chem. Soc., 116(22), 9901-11 (English) 1994. CODEN: JACSAT. ISSN: 0002-7863.

GI



I

AB A new class of phosphorylated nucleosides,, e.g. I (R = Na, Et), were synthesized in good yields via phosphitylation of the amino group of appropriately protected adenosine derivs. In a similar manner, cytidine 4-N-phosphoramidate (4-N-CMP), guanosine 2-N-phosphoramidate (2-N-GMP), and their di-Et ester derivs. were synthesized. These new compds. were characterized by ¹H, ¹³C, and ³¹P NMR, UV, CD, IR, electrophoresis, and mass spectroscopy. The conformation and water soly. of these N-phosphorylated ribonucleoside derivs. have been studied in detail.

L5 ANSWER 25 OF 140 REGISTRY COPYRIGHT 2002 ACS

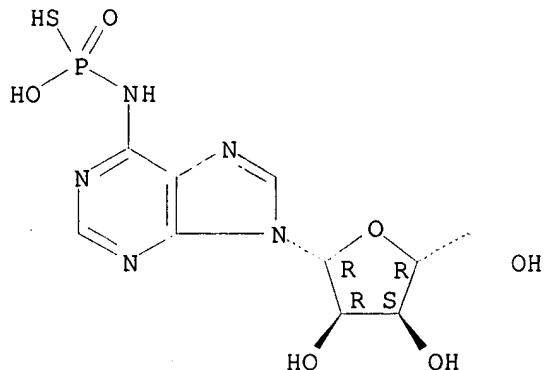
RN 161879-75-0 REGISTRY

CN Phosphoramidothioic acid, (9-.beta.-D-ribofuranosyl-9H-purin-6-yl)-,

Searched by: Mary Hale 308-4258 CM-1 1E01

disodium salt (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C10 H14 N5 O6 P S . 2 Na
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.

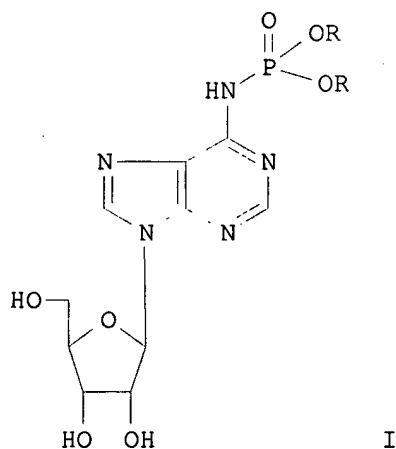


● 2 Na

1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 122:214406 Synthesis and Properties of N-Phosphorylated Ribonucleosides. Wada, Takeshi; Moriguchi, Tomohisa; Sekine, Mitsuo (Faculty of Bioscience and Biotechnology, Tokyo Institute of Technology, Yokohama, 227, Japan). J. Am. Chem. Soc., 116(22), 9901-11 (English) 1994. CODEN: JACSAT. ISSN: 0002-7863.

GI



I

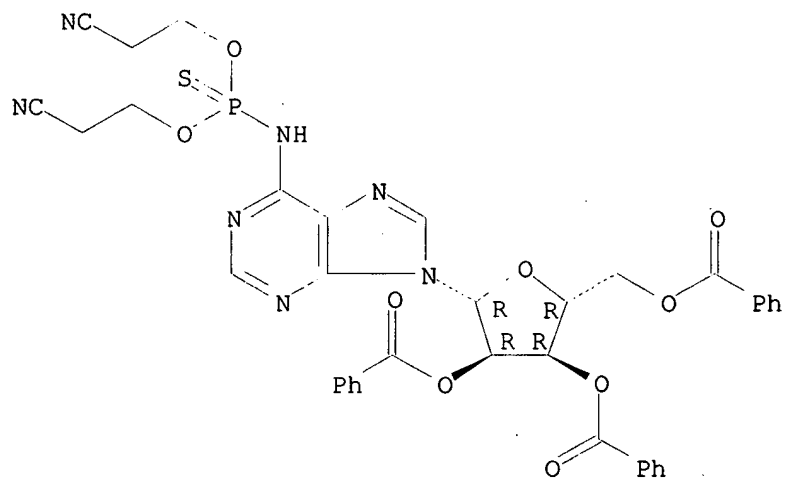
AB A new class of phosphorylated nucleosides,, e.g. I (R = Na, Et), were synthesized in good yields via phosphitylation of the amino group of appropriately protected adenosine derivs. In a similar manner, cytidine 4-N-phosphoramidate (4-N-CMP), guanosine 2-N-phosphoramidate (2-N-GMP), and their di-Et ester derivs. were synthesized. These new compds. were

Searched by: Mary Hale 308-4258 CM-1 1E01

characterized by ^1H , ^{13}C , and ^{31}P NMR, UV, CD, IR, electrophoresis, and mass spectroscopy. The conformation and water soly. of these N-phosphorylated ribonucleoside derivs. have been studied in detail.

L5 ANSWER 26 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 161879-74-9 REGISTRY
CN Phosphoramidothioic acid, [9-(2,3,5-tri-O-benzoyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, O,O-bis(2-cyanoethyl) ester (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C37 H32 N7 O9 P S
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

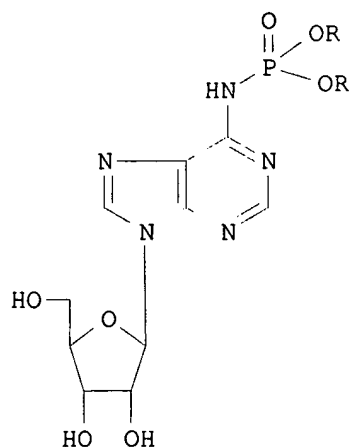


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 122:214406 Synthesis and Properties of N-Phosphorylated Ribonucleosides. Wada, Takeshi; Moriguchi, Tomohisa; Sekine, Mitsuo (Faculty of Bioscience and Biotechnology, Tokyo Institute of Technology, Yokohama, 227, Japan). J. Am. Chem. Soc., 116(22), 9901-11 (English) 1994. CODEN: JACSAT. ISSN: 0002-7863.

GI



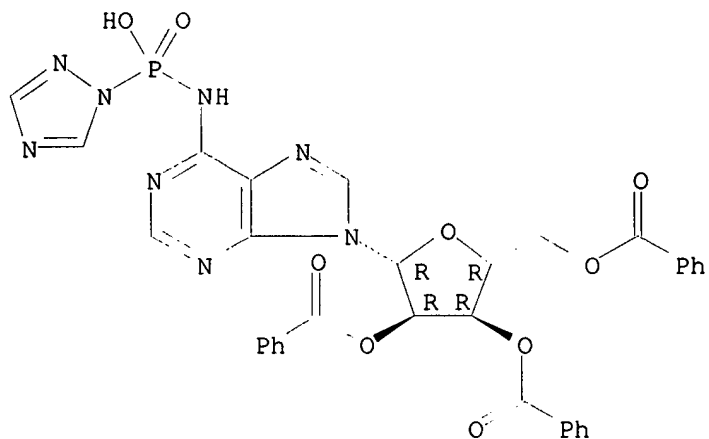
AB A new class of phosphorylated nucleosides,, e.g. I (R = Na, Et), were synthesized in good yields via phosphitylation of the amino group of appropriately protected adenosine derivs. In a similar manner, cytidine 4-N-phosphoramidate (4-N-CMP), guanosine 2-N-phosphoramidate (2-N-GMP), and their di-Et ester derivs. were synthesized. These new compds. were characterized by ¹H, ¹³C, and ³¹P NMR, UV, CD, IR, electrophoresis, and mass spectroscopy. The conformation and water soly. of these N-phosphorylated ribonucleoside derivs. have been studied in detail.

L5 ANSWER 27 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 161879-73-8 REGISTRY
 CN Phosphonamidic acid, P-1H-1,2,4-triazol-1-yl-N-[9-(2,3,5-tri-O-benzoyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C33 H27 N8 O9 P . C6 H15 N
 SR CA
 LC STN Files: CA, CAPLUS

CM 1

CRN 161879-72-7
 CMF C33 H27 N8 O9 P

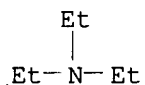
Absolute stereochemistry.



CM 2

CRN 121-44-8

CMF C6 H15 N

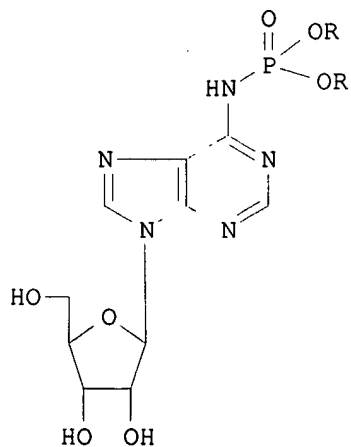


1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 122:214406 Synthesis and Properties of N-Phosphorylated Ribonucleosides. Wada, Takeshi; Moriguchi, Tomohisa; Sekine, Mitsuo (Faculty of Bioscience and Biotechnology, Tokyo Institute of Technology, Yokohama, 227, Japan). J. Am. Chem. Soc., 116(22), 9901-11 (English) 1994. CODEN: JACSAT. ISSN: 0002-7863.

GI



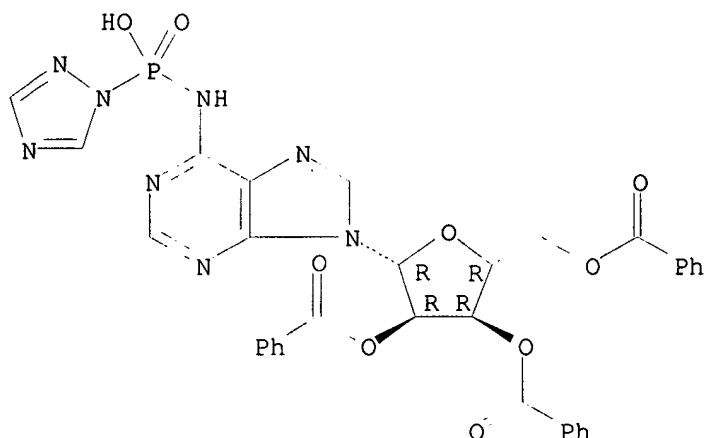
I

Searched by: Mary Hale 308-4258 CM-1 1E01

AB A new class of phosphorylated nucleosides,, e.g. I (R = Na, Et), were synthesized in good yields via phosphitylation of the amino group of appropriately protected adenosine derivs. In a similar manner, cytidine 4-N-phosphoramidate (4-N-CMP), guanosine 2-N-phosphoramidate (2-N-GMP), and their di-Et ester derivs. were synthesized. These new compds. were characterized by ¹H, ¹³C, and ³¹P NMR, UV, CD, IR, electrophoresis, and mass spectroscopy. The conformation and water soly. of these N-phosphorylated ribonucleoside derivs. have been studied in detail.

L5 ANSWER 28 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 161879-72-7 REGISTRY
CN Phosphoramidic acid, P-1H-1,2,4-triazol-1-yl-N-[9-(2,3,5-tri-O-benzoyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C33 H27 N8 O9 P
CI COM
SR CA

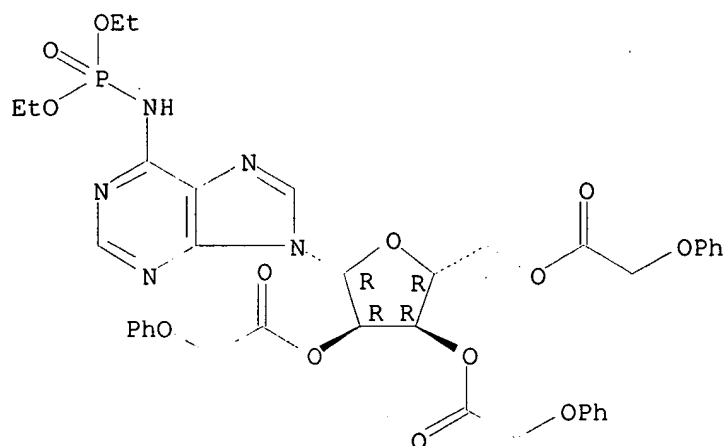
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 29 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 154986-10-4 REGISTRY
CN Phosphoramidic acid, [9-[2,3,5-tris-O-(phenoxyacetyl)-.beta.-D-ribofuranosyl]-9H-purin-6-yl]-, diethyl ester (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Acetic acid, phenoxy-, triester with diethyl (9-.beta.-D-ribofuranosyl-9H-purin-6-yl)phosphoramidate
FS STEREOSEARCH
MF C38 H40 N5 O13 P
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



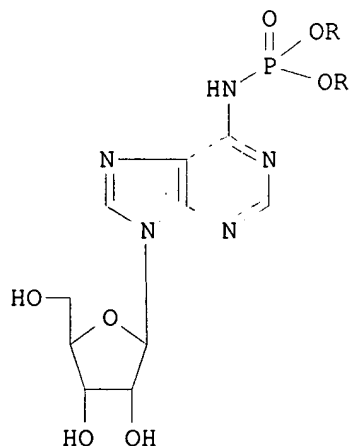
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)

2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 122:214406 Synthesis and Properties of N-Phosphorylated Ribonucleosides. Wada, Takeshi; Moriguchi, Tomohisa; Sekine, Mitsuo (Faculty of Bioscience and Biotechnology, Tokyo Institute of Technology, Yokohama, 227, Japan). J. Am. Chem. Soc., 116(22), 9901-11 (English) 1994. CODEN: JACSAT. ISSN: 0002-7863.

GI



I

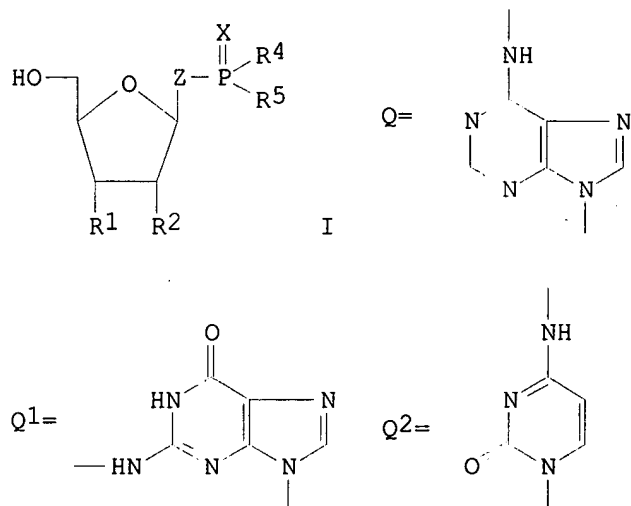
AB A new class of phosphorylated nucleosides,, e.g. I (R = Na, Et), were synthesized in good yields via phosphitylation of the amino group of appropriately protected adenosine derivs. In a similar manner, cytidine 4-N-phosphoramidate (4-N-CMP), guanosine 2-N-phosphoramidate (2-N-GMP), and their di-Et ester derivs. were synthesized. These new compds. were characterized by ¹H, ¹³C, and ³¹P NMR, UV, CD, IR, electrophoresis, and mass spectroscopy. The conformation and water soly. of these N-phosphorylated ribonucleoside derivs. have been studied in detail.

REFERENCE 2: 120:324143 Preparation of nucleic acid-related compounds.

Searched by: Mary Hale 308-4258 CM-1 1E01

Sekine, Mitsuo; Wada, Takeshi (Wako Pure Chem Ind Ltd, Japan). Jpn. Kokai Tokkyo Koho JP 06009681 A2 19940118 Heisei, 11 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1993-76085 19930310. PRIORITY: JP 1992-88134 19920312.

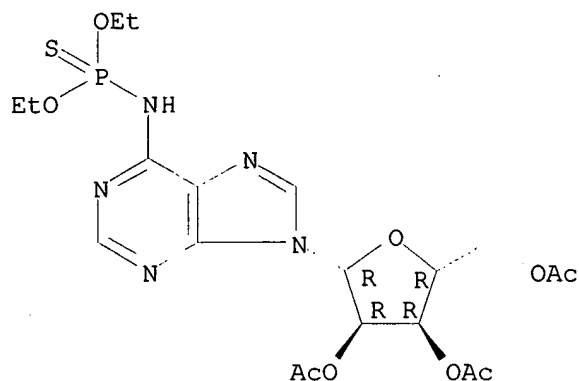
GI



AB Nucleoside N-(thio)phosphoramidate derivs. [I; R1, R2 = H, OH; Z = Q - Q2; X = O, S, Se; R4, R5 = OH, NH2, (un)substituted C1-18 alkoxy or aryloxy], useful as pharmaceuticals, agrochems., and medical diagnostic agents (no data), are prepd. Thus, 1,2,4-1H-triazole was dissolved in acetone and reacted with P(O)Cl3 and Et3N at 0.degree. for 30 min and then with a soln. of 2',3',5'-tri-O-benzoyl-adenosine in MeCN to give 80% triethylammonium 2',3',5'-tri-O-benzoyl-adenosine-6-N-(triazolyl)phosphoramidate, which was treated with concd. aq. NH3-pyridine mixt. to give, after purifn. by anion exchange chromatog. using DEA cellulose and lyophilization, 83% triethylammonium adenosine-6-N-(amino)phosphoramidate.

L5 ANSWER 30 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 154971-69-4 REGISTRY
 CN Phosphoramidothioic acid, [9-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, O,O-diethyl ester (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C20 H28 N5 O9 P S
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.



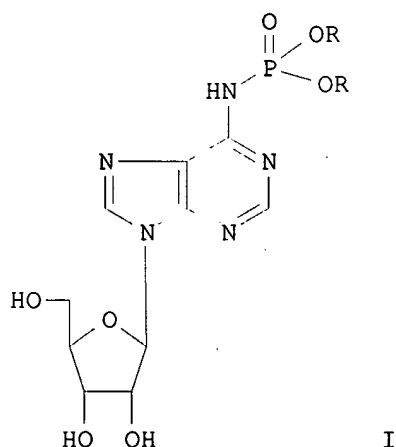
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)

2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 122:214406 Synthesis and Properties of N-Phosphorylated Ribonucleosides. Wada, Takeshi; Moriguchi, Tomohisa; Sekine, Mitsuo (Faculty of Bioscience and Biotechnology, Tokyo Institute of Technology, Yokohama, 227, Japan). J. Am. Chem. Soc., 116(22), 9901-11 (English) 1994. CODEN: JACSAT. ISSN: 0002-7863.

GI



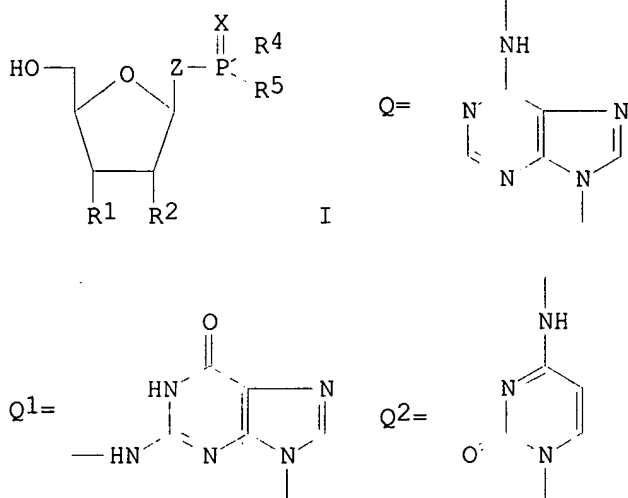
I

AB A new class of phosphorylated nucleosides,, e.g. I (R = Na, Et), were synthesized in good yields via phosphitylation of the amino group of appropriately protected adenosine derivs. In a similar manner, cytidine 4-N-phosphoramidate (4-N-CMP), guanosine 2-N-phosphoramidate (2-N-GMP), and their di-Et ester derivs. were synthesized. These new compds. were characterized by ¹H, ¹³C, and ³¹P NMR, UV, CD, IR, electrophoresis, and mass spectroscopy. The conformation and water soly. of these N-phosphorylated ribonucleoside derivs. have been studied in detail.

REFERENCE 2: 120:324143 Preparation of nucleic acid-related compounds. Sekine, Mitsuo; Wada, Takeshi (Wako Pure Chem Ind Ltd, Japan). Jpn. Kokai Tokkyo Koho JP 06009681 A2 19940118 Heisei, 11 pp. (Japanese). CODEN:

Searched by: Mary Hale 308-4258 CM-1 1E01

GI



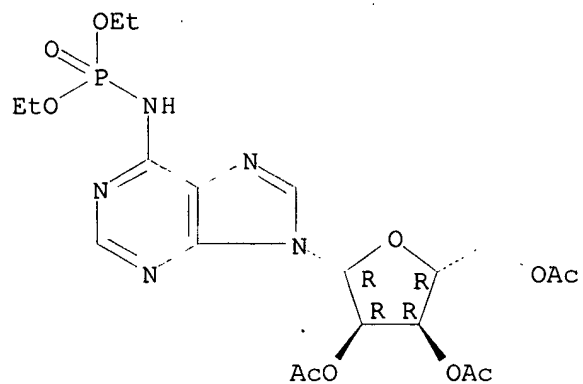
AB Nucleoside N-(thio)phosphoramidate derivs. [I; R1, R2 = H, OH; Z = Q - Q2; X = O, S, Se; R4, R5 = OH, NH2, (un)substituted C1-18 alkoxy or aryloxy], useful as pharmaceuticals, agrochems., and medical diagnostic agents (no data), are prepd. Thus, 1,2,4-1H-triazole was dissolved in acetone and reacted with P(O)Cl3 and Et3N at 0.degree. for 30 min and then with a soln. of 2',3',5'-tri-O-benzoyladenosine in MeCN to give 80% triethylammonium 2',3',5'-tri-O-benzoyladenosine-6-N-(triazolyl)phosphoramidate, which was treated with concd. aq. NH3-pyridine mixt. to give, after purifn. by anion exchange chromatog. using DEA cellulose and lyophilization, 83% triethylammonium adenosine-6-N-(amino)phosphoramidate.

L5 ANSWER 31 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 154971-67-2 REGISTRY
CN Phosphoramidic acid, [9-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, diethyl ester, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C20 H28 N5 O10 P . C6 H15 N
SR CA
LC STN Files: CA, CAPLUS

CM 1

CRN 154534-46-0
CMF C20 H28 N5 O10 P

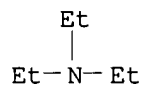
Absolute stereochemistry.



CM 2

CRN 121-44-8

CMF C6 H15 N

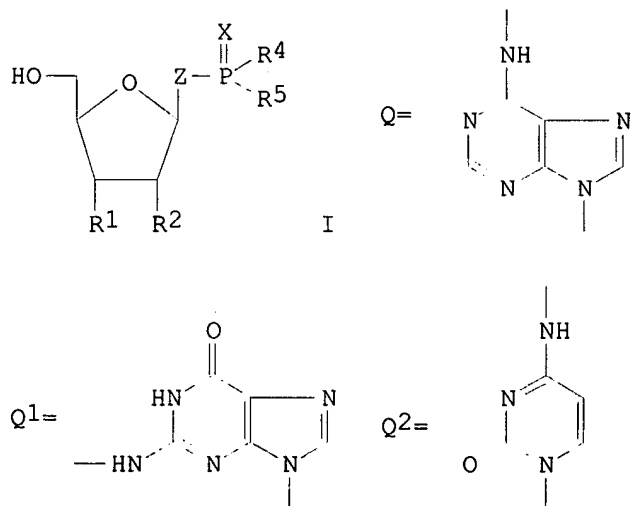


1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 120:324143 Preparation of nucleic acid-related compounds.
 Sekine, Mitsuo; Wada, Takeshi (Wako Pure Chem Ind Ltd, Japan). Jpn. Kokai
 Tokkyo Koho JP 06009681 A2 19940118 Heisei, 11 pp. (Japanese). CODEN:
 JKXXAF. APPLICATION: JP 1993-76085 19930310. PRIORITY: JP 1992-88134
 19920312.

GI



AB Nucleoside N-(thio)phosphoramidate derivs. [I; R1, R2 = H, OH; Z = Q - Q2; X = O, S, Se; R4, R5 = OH, NH2, (un)substituted C1-18 alkoxy or aryloxy], useful as pharmaceuticals, agrochems., and medical diagnostic agents (no data), are prepd. Thus, 1,2,4-1H-triazole was dissolved in acetone and reacted with P(O)Cl3 and Et3N at 0.degree. for 30 min and then with a soln. of 2',3',5'-tri-O-benzoyladenosine in MeCN to give 80% triethylammonium 2',3',5'-tri-O-benzoyladenosine-6-N-(triazolyl)phosphoramidate, which was treated with concd. aq. NH3-pyridine mixt. to give, after purifn. by anion exchange chromatog. using DEA cellulose and lyophilization, 83% triethylammonium adenosine-6-N-(amino)phosphoramidate.

L5 ANSWER 32 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 154971-66-1 REGISTRY

CN Phosphoramidic acid, (9-.beta.-D-ribofuranosyl-9H-purin-6-yl)-, disodium salt (9CI) (CA INDEX NAME)

OTHER NAMES:

CN Disodium adenosine-6-N-phosphoramidate

FS STEREOSEARCH

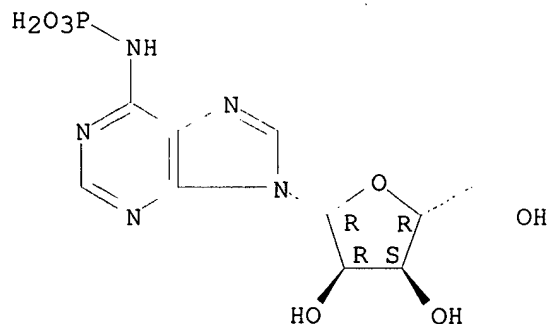
MF C10 H14 N5 O7 P . 2 Na

SR CA

LC STN Files: CA, CAPLUS

CRN (83305-95-7)

Absolute stereochemistry.



● 2 Na

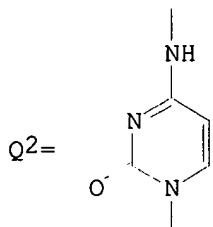
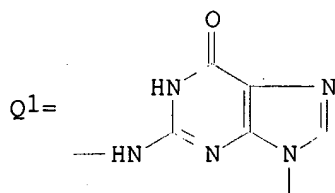
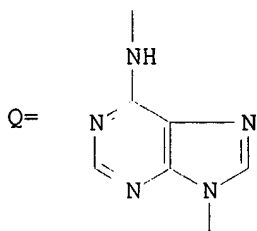
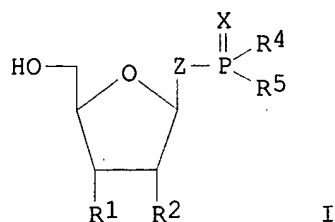
1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 120:324143 Preparation of nucleic acid-related compounds. Sekine, Mitsuo; Wada, Takeshi (Wako Pure Chem Ind Ltd, Japan). Jpn. Kokai Tokkyo Koho JP 06009681 A2 19940118 Heisei, 11 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1993-76085 19930310. PRIORITY: JP 1992-88134 19920312.

GI

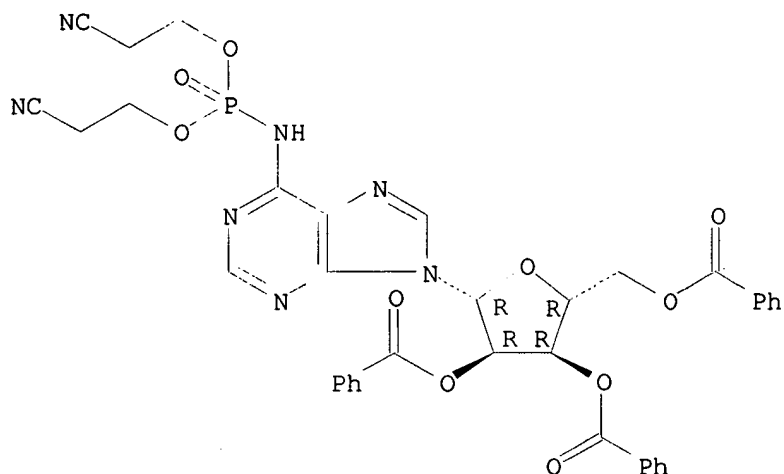
Searched by: Mary Hale 308-4258 CM-1 1E01



AB Nucleoside N-(thio)phosphoramidate derivs. [I; R1, R2 = H, OH; Z = Q - Q2; X = O, S, Se; R4, R5 = OH, NH2, (un)substituted C1-18 alkoxy or aryloxy], useful as pharmaceuticals, agrochems., and medical diagnostic agents (no data), are prepd. Thus, 1,2,4-1H-triazole was dissolved in acetone and reacted with P(O)Cl3 and Et3N at 0.degree. for 30 min and then with a soln. of 2',3',5'-tri-O-benzoyl-adenosine in MeCN to give 80% triethylammonium 2',3',5'-tri-O-benzoyl-adenosine-6-N-(triazolyl)phosphoramidate, which was treated with concd. aq. NH3-pyridine mixt. to give, after purifn. by anion exchange chromatog. using DEA cellulose and lyophilization, 83% triethylammonium adenosine-6-N-(amino)phosphoramidate.

L5 ANSWER 33 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 154971-65-0 REGISTRY
 CN Phosphoramidic acid, [9-(2,3,5-tri-O-benzoyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, bis(2-cyanoethyl) ester (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C37 H32 N7 O10 P
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.



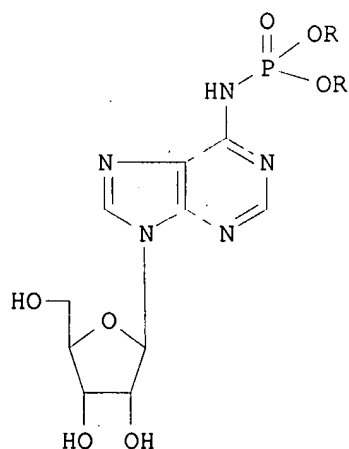
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)

2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 122:214406 Synthesis and Properties of N-Phosphorylated Ribonucleosides. Wada, Takeshi; Moriguchi, Tomohisa; Sekine, Mitsuo (Faculty of Bioscience and Biotechnology, Tokyo Institute of Technology, Yokohama, 227, Japan). J. Am. Chem. Soc., 116(22), 9901-11 (English) 1994. CODEN: JACSAT. ISSN: 0002-7863.

GI

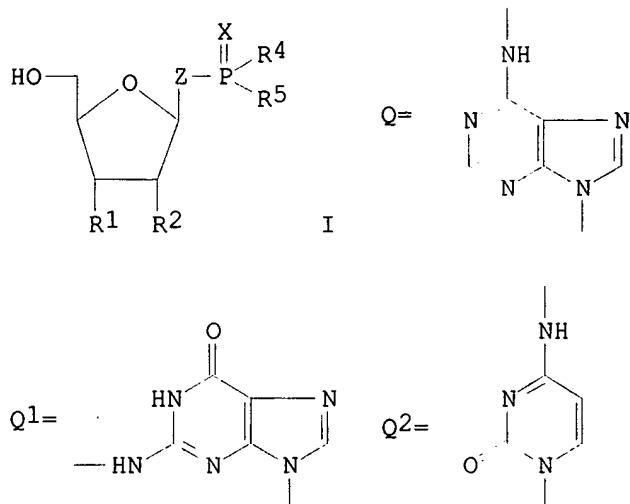


I

AB A new class of phosphorylated nucleosides,, e.g. I (R = Na, Et), were synthesized in good yields via phosphitylation of the amino group of appropriately protected adenosine derivs. In a similar manner, cytidine 4-N-phosphoramidate (4-N-CMP), guanosine 2-N-phosphoramidate (2-N-GMP), and their di-Et ester derivs. were synthesized. These new compds. were characterized by ¹H, ¹³C, and ³¹P NMR, UV, CD, IR, electrophoresis, and mass spectroscopy. The conformation and water soly. of these N-phosphorylated ribonucleoside derivs. have been studied in detail.

REFERENCE 2: 120:324143 Preparation of nucleic acid-related compounds.
 Sekine, Mitsuo; Wada, Takeshi (Wako Pure Chem Ind Ltd, Japan). Jpn. Kokai
 Tokkyo Koho JP 06009681 A2 19940118 Heisei, 11 pp. (Japanese). CODEN:
 JKXXAF. APPLICATION: JP 1993-76085 19930310. PRIORITY: JP 1992-88134
 19920312.

GI



AB Nucleoside N-(thio)phosphoramidate derivs. [I; R1, R2 = H, OH; Z = Q - Q2; X = O, S, Se; R4, R5 = OH, NH2, (un)substituted C1-18 alkoxy or aryloxy], useful as pharmaceuticals, agrochems., and medical diagnostic agents (no data), are prepd. Thus, 1,2,4-1H-triazole was dissolved in acetone and reacted with P(O)Cl3 and Et3N at 0.degree. for 30 min and then with a soln. of 2',3',5'-tri-O-benzoyladenosine in MeCN to give 80% triethylammonium 2',3',5'-tri-O-benzoyladenosine-6-N-(triazolyl)phosphoramidate, which was treated with concd. aq. NH3-pyridine mixt. to give, after purifn. by anion exchange chromatog. using DEA cellulose and lyophilization, 83% triethylammonium adenosine-6-N-(amino)phosphoramidate.

L5 ANSWER 34 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 154971-64-9 REGISTRY

CN Phosphoramidic acid, (9-.beta.-D-ribofuranosyl-9H-purin-6-yl)-, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

OTHER NAMES:

CN Triethylammonium adenosine-6-N-phosphoramidate

FS STEREOSEARCH

MF C10 H14 N5 O7 P . C6 H15 N

SR CA

LC STN Files: CA, CAPLUS

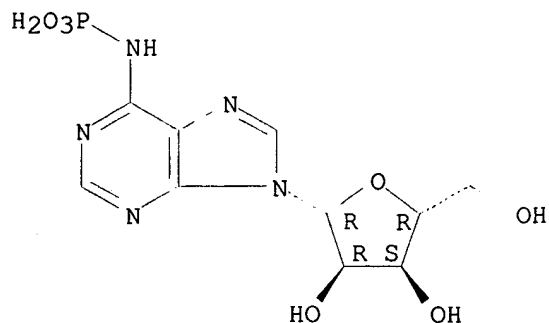
CM 1

CRN 83305-95-7

CMF C10 H14 N5 O7 P

Absolute stereochemistry.

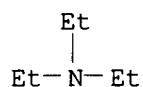
Searched by: Mary Hale 308-4258 CM-1 1E01



CM 2

CRN 121-44-8

CMF C6 H15 N

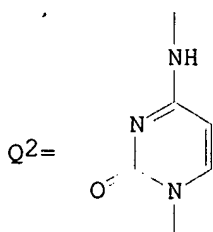
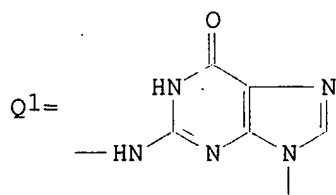
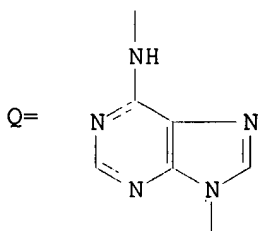
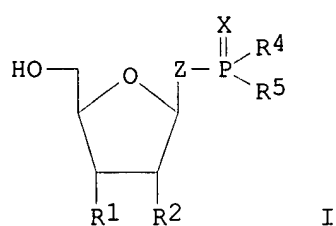


1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 120:324143 Preparation of nucleic acid-related compounds.
 Sekine, Mitsuo; Wada, Takeshi (Wako Pure Chem Ind Ltd, Japan). Jpn. Kokai
 Tokkyo Koho JP 06009681 A2 19940118 Heisei, 11 pp. (Japanese). CODEN:
 JKXXAF. APPLICATION: JP 1993-76085 19930310. PRIORITY: JP 1992-88134
 19920312.

GI



AB Nucleoside N-(thio)phosphoramidate derivs. [I; R1, R2 = H, OH; Z = Q - Q2;

Searched by: Mary Hale 308-4258 CM-1 1E01

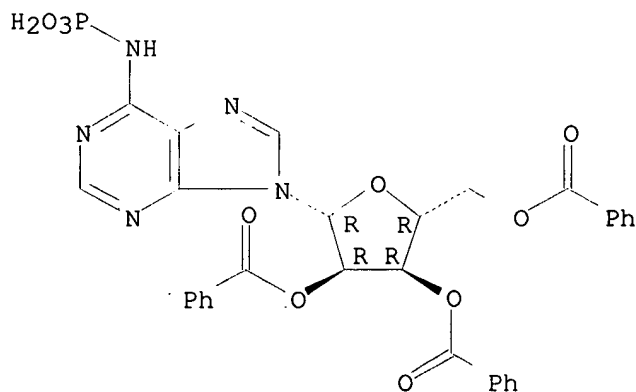
X = O, S, Se; R4, R5 = OH, NH2, (un)substituted C1-18 alkoxy or aryloxy], useful as pharmaceuticals, agrochemicals, and medical diagnostic agents (no data), are prepared. Thus, 1,2,4-triazole was dissolved in acetone and reacted with P(O)Cl3 and Et3N at 0 degree for 30 min and then with a soln. of 2',3',5'-tri-O-benzoyl-adenosine in MeCN to give 80% triethylammonium 2',3',5'-tri-O-benzoyl-adenosine-6-N-(triazolyl)phosphoramidate, which was treated with concd. aq. NH3-pyridine mixt. to give, after purification by anion exchange chromatography using DEA cellulose and lyophilization, 83% triethylammonium adenosine-6-N-(amino)phosphoramidate.

L5 ANSWER 35 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 154971-63-8 REGISTRY
 CN Phosphoramidic acid, [9-(2,3,5-tri-O-benzoyl-beta.-D-ribofuranosyl)-9H-purin-6-yl]-, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C31 H26 N5 O10 P . C6 H15 N
 SR CA
 LC STN Files: CA, CAPLUS

CM 1

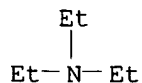
CRN 154971-62-7
 CMF C31 H26 N5 O10 P

Absolute stereochemistry.



CM 2

CRN 121-44-8
 CMF C6 H15 N

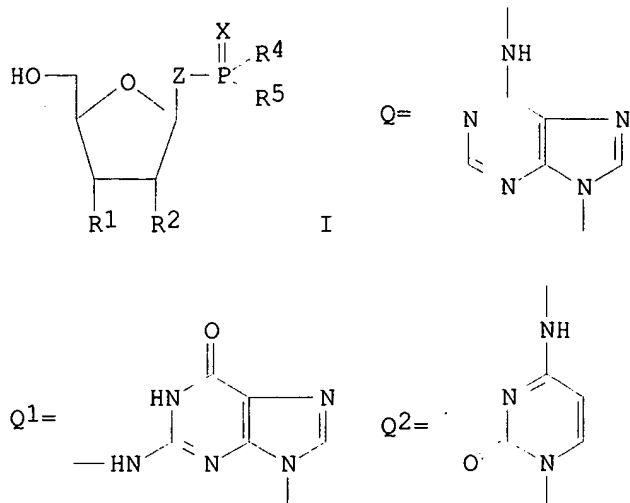


1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 120:324143 Preparation of nucleic acid-related compounds.
 Sekine, Mitsuo; Wada, Takeshi (Wako Pure Chem Ind Ltd, Japan). Jpn. Kokai
 Tokkyo Koho JP 06009681 A2 19940118 Heisei, 11 pp. (Japanese). CODEN:

Searched by: Mary Hale 308-4258 CM-1 1E01

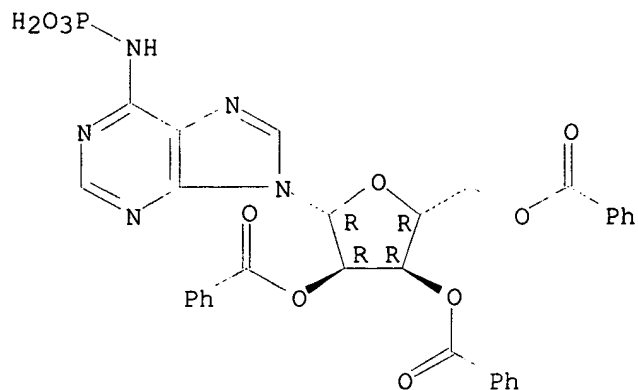
GI



AB Nucleoside N-(thio)phosphoramidate derivs. [I; R1, R2 = H, OH; Z = Q - Q2; X = O, S, Se; R4, R5 = OH, NH2, (un)substituted C1-18 alkoxy or aryloxy], useful as pharmaceuticals, agrochems., and medical diagnostic agents (no data), are prepd. Thus, 1,2,4-1H-triazole was dissolved in acetone and reacted with P(O)Cl3 and Et3N at 0.degree. for 30 min and then with a soln. of 2',3',5'-tri-O-benzoyl-adenosine in MeCN to give 80% triethylammonium 2',3',5'-tri-O-benzoyl-adenosine-6-N-(triazolyl)phosphoramidate, which was treated with concd. aq. NH3-pyridine mixt. to give, after purifn. by anion exchange chromatog. using DEA cellulose and lyophilization, 83% triethylammonium adenosine-6-N-(amino)phosphoramidate.

L5 ANSWER 36 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 154971-62-7 REGISTRY
CN Phosphoramidic acid, [9-(2,3,5-tri-O-benzoyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C31 H26 N5 O10 P
CI COM
SR CA

Absolute stereochemistry.



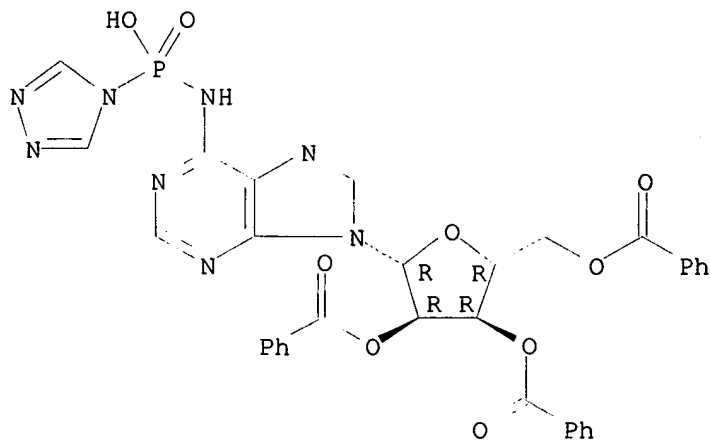
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 37 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 154971-61-6 REGISTRY
 CN Phosphonamidic acid, P-4H-1,2,4-triazol-4-yl-N-[9-(2,3,5-tri-O-benzoyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C33 H27 N8 O9 P . C6 H15 N
 SR CA
 LC STN Files: CA, CAPLUS

CM 1

CRN 154971-60-5
 CMF C33 H27 N8 O9 P

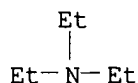
Absolute stereochemistry.



CM 2

CRN 121-44-8
 CMF C6 H15 N

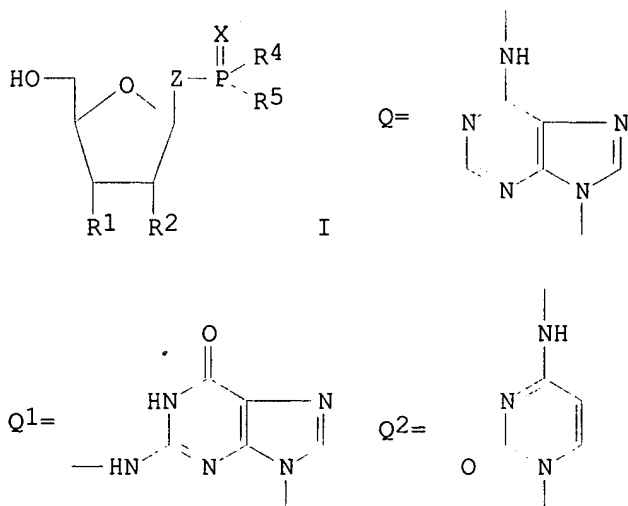
Searched by: Mary Hale 308-4258 CM-1 1E01



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 120:324143 Preparation of nucleic acid-related compounds.
Sekine, Mitsuo; Wada, Takeshi (Wako Pure Chem Ind Ltd, Japan). Jpn. Kokai
Tokkyo Koho JP 06009681 A2 19940118 Heisei, 11 pp. (Japanese). CODEN:
JKXXAF. APPLICATION: JP 1993-76085 19930310. PRIORITY: JP 1992-88134
19920312.

GI

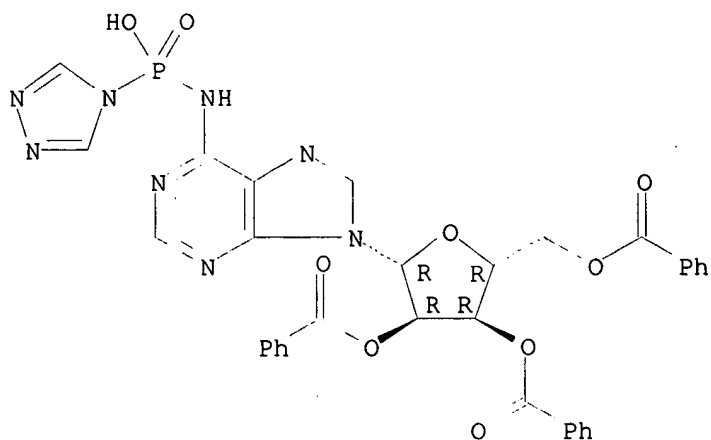


AB Nucleoside N-(thio)phosphoramidate derivs. [I; R1, R2 = H, OH; Z = Q - Q2; X = O, S, Se; R4, R5 = OH, NH2, (un)substituted C1-18 alkoxy or aryloxy], useful as pharmaceuticals, agrochems., and medical diagnostic agents (no data), are prepd. Thus, 1,2,4-1H-triazole was dissolved in acetone and reacted with P(O)Cl3 and Et3N at 0.degree. for 30 min and then with a soln. of 2',3',5'-tri-O-benzoyl-adenosine in MeCN to give 80% triethylammonium 2',3',5'-tri-O-benzoyl-adenosine-6-N-(triazolyl)phosphoramidate, which was treated with concd. aq. NH3-pyridine mixt. to give, after purifn. by anion exchange chromatog. using DEA cellulose and lyophilization, 83% triethylammonium adenosine-6-N-(amino)phosphoramidate.

L5 ANSWER 38 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 154971-60-5 REGISTRY
CN Phosphonamidic acid, P-4H-1,2,4-triazol-4-yl-N-[9-(2,3,5-tri-O-benzoyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C33 H27 N8 O9 P
CI COM
SR CA

Absolute stereochemistry.

Searched by: Mary Hale 308-4258 CM-1 1E01



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 39 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 154971-59-2 REGISTRY
 CN Phosphorodiamidic acid, (9-.beta.-D-ribofuranosyl-9H-purin-6-yl)-, compd.
 with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

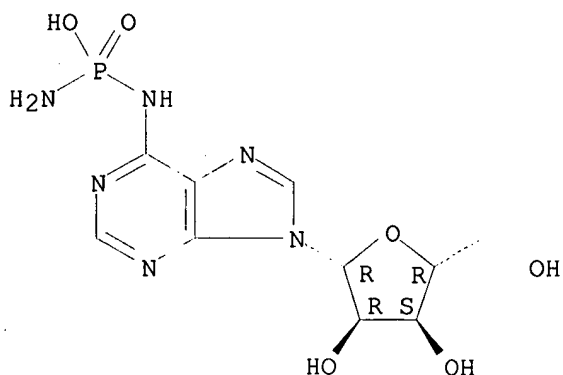
OTHER NAMES:

CN Triethylammonium adenosine-6-N-(amino)phosphoramidate
 FS STEREOSEARCH
 MF C10 H15 N6 O6 P . C6 H15 N
 SR CA
 LC STN Files: CA, CAPLUS

CM 1

CRN 154971-58-1
 CMF C10 H15 N6 O6 P

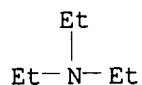
Absolute stereochemistry.



CM 2

CRN 121-44-8
 CMF C6 H15 N

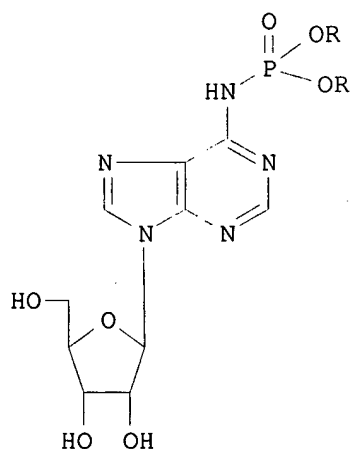
Searched by: Mary Hale 308-4258 CM-1 1E01



2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 122:214406 Synthesis and Properties of N-Phosphorylated Ribonucleosides. Wada, Takeshi; Moriguchi, Tomohisa; Sekine, Mitsuo (Faculty of Bioscience and Biotechnology, Tokyo Institute of Technology, Yokohama, 227, Japan). J. Am. Chem. Soc., 116(22), 9901-11 (English) 1994. CODEN: JACSAT. ISSN: 0002-7863.

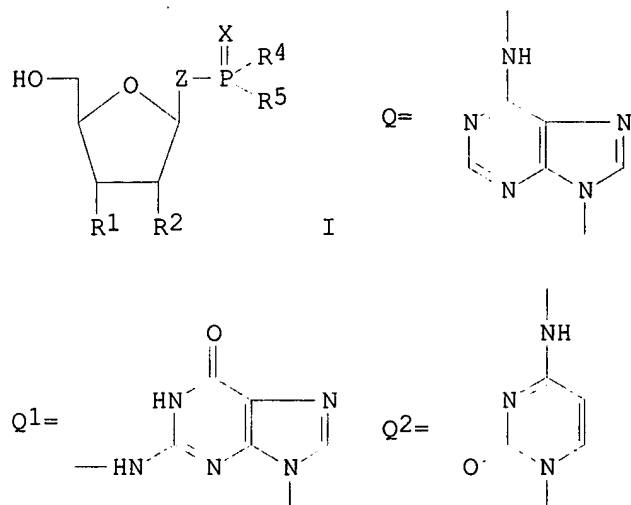
GI



AB A new class of phosphorylated nucleosides,, e.g. I (R = Na, Et), were synthesized in good yields via phosphitylation of the amino group of appropriately protected adenosine derivs. In a similar manner, cytidine 4-N-phosphoramidate (4-N-CMP), guanosine 2-N-phosphoramidate (2-N-GMP), and their di-Et ester derivs. were synthesized. These new compds. were characterized by ¹H, ¹³C, and ³¹P NMR, UV, CD, IR, electrophoresis, and mass spectroscopy. The conformation and water soly. of these N-phosphorylated ribonucleoside derivs. have been studied in detail.

REFERENCE 2: 120:324143 Preparation of nucleic acid-related compounds. Sekine, Mitsuo; Wada, Takeshi (Wako Pure Chem Ind Ltd, Japan). Jpn. Kokai Tokkyo Koho JP 06009681 A2 19940118 Heisei, 11 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1993-76085 19930310. PRIORITY: JP 1992-88134 19920312.

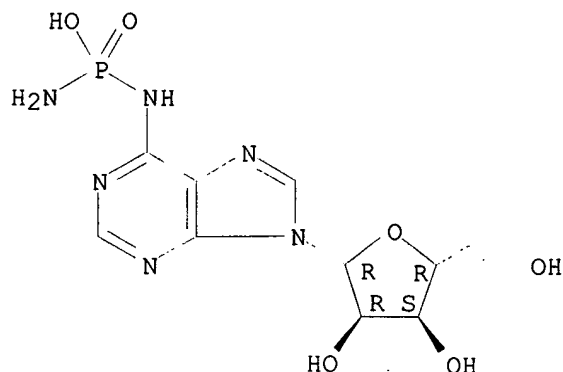
GI



AB Nucleoside N-(thio)phosphoramidate derivs. [I; R1, R2 = H, OH; Z = Q - Q2; X = O, S, Se; R4, R5 = OH, NH2, (un)substituted C1-18 alkoxy or aryloxy], useful as pharmaceuticals, agrochems., and medical diagnostic agents (no data), are prepd. Thus, 1,2,4-1H-triazole was dissolved in acetone and reacted with P(O)Cl3 and Et3N at 0.degree. for 30 min and then with a soln. of 2',3',5'-tri-O-benzoyl-adenosine in MeCN to give 80% triethylammonium 2',3',5'-tri-O-benzoyl-adenosine-6-N-(triazolyl)phosphoramidate, which was treated with concd. aq. NH3-pyridine mixt. to give, after purifn. by anion exchange chromatog. using DEA cellulose and lyophilization, 83% triethylammonium adenosine-6-N-(amino)phosphoramidate.

L5 ANSWER 40 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 154971-58-1 REGISTRY
 CN Phosphorodiamidic acid, (9-.beta.-D-ribofuranosyl-9H-purin-6-yl)- (9CI)
 (CA INDEX NAME)
 FS STEREOSEARCH
 MF C10 H15 N6 O6 P
 CI COM
 SR CA

Absolute stereochemistry.

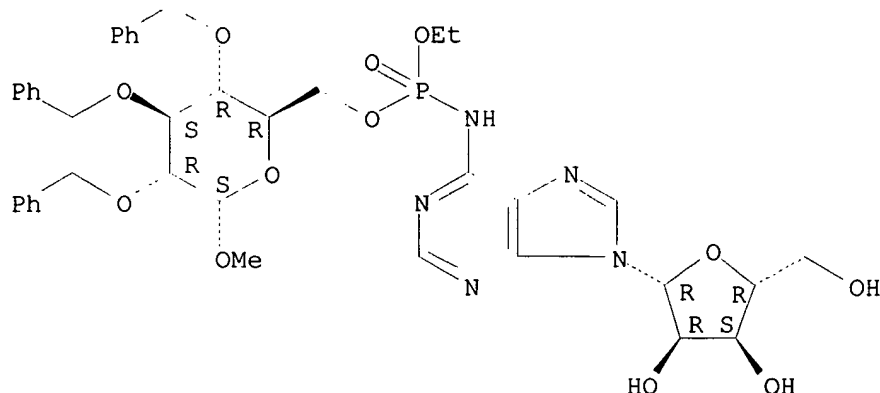


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

Searched by: Mary Hale 308-4258 CM-1 1E01

L5 ANSWER 41 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 154534-49-3 REGISTRY
 CN .alpha.-D-Glucopyranoside, methyl 2,3,4-tris-O-(phenylmethyl)-, ethyl
 (9-.beta.-D-ribofuranosyl-9H-purin-6-yl)phosphoramidate (9CI) (CA INDEX
 NAME)
 FS STEREOSEARCH
 MF C40 H48 N5 O12 P
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.

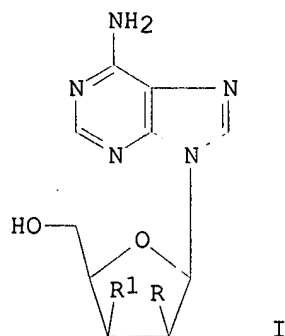


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 120:271041 Nucleic acid related compounds. 81. Syntheses of 9-(3-deoxy-.beta.-D-threo-pentofuranosyl)adenine, the core nucleoside of the extraordinarily selective antibiotic agrocin 84, and simplified structural component analogs. Vinayak, Ravi; Hansske, Fritz; Robins, Morris J. (Dep. Chem., Univ. Alberta, Edmonton, AB, Can.). J. Heterocycl. Chem., 30(5), 1181-9 (English) 1993. CODEN: JHTCAD. ISSN: 0022-152X.

GI



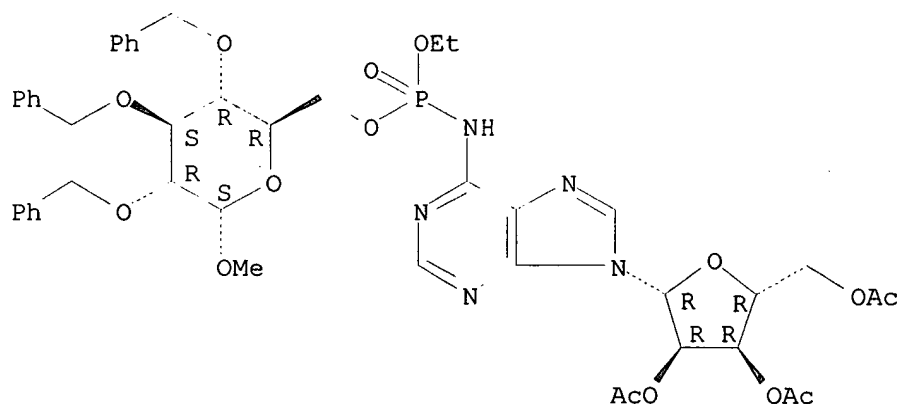
AB Alternative syntheses of (deoxy-.beta.-D-threo-pentofuranosyl)adenine I (R = OH, R1 = H) (II), the core nucleoside of agrocin 84 and its 2'-deoxy

Searched by: Mary Hale 308-4258 CM-1 1E01

threo isomer I (R = H, R1 = OH) (III) were devised: (1) direct conversion of 9-(.beta.-D-arabinofuranosyl)adenine into 9-(2,3-anhydro-.beta.-D-lyxofuranosyl)adenine and regioselective opening of its oxirane ring with sodium borohydride to give II and III (.apprx.7.5:1); (2) treatment of adenosine with sodium hydride and 2,4,6-triisopropylbenzenesulfonyl chloride, and subjection of the resulting 2'(3')-sulfonates to the reductive [1,2]-hydride shift rearrangement with lithium triethylborohydride to give II and III (.apprx.2:1); and (3) subjection of the phenoxythiocarbonyl esters of 9-[2(3),5-bis-O-(tert-butyldimethylsilyl)-.beta.-D-arabinofuranosyl]adenine to Barton deoxygenation, and deprotection to give II and 2'-deoxyadenosine (.apprx.5:1). Methods (2) and (3) gave lower yields. Syntheses of simplified 6-N- and 5'-O-adenosine phosphoramidate model compds. were explored to examine potential access to such features in the structure proposed for agrocin 84.

L5 ANSWER 42 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 154534-48-2 REGISTRY
 CN .alpha.-D-Glucopyranoside, methyl 2,3,4-tris-O-(phenylmethyl)-, ethyl [9-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]phosphoramidate (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C46 H54 N5 O15 P
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.



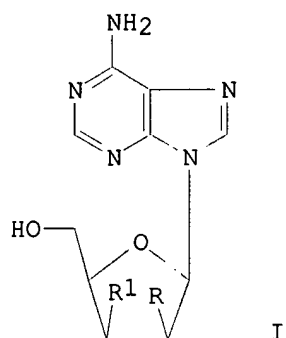
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 120:271041 Nucleic acid related compounds. 81. Syntheses of 9-(3-deoxy-.beta.-D-threo-pentofuranosyl)adenine, the core nucleoside of the extraordinarily selective antibiotic agrocin 84, and simplified structural component analogs. Vinayak, Ravi; Hansske, Fritz; Robins, Morris J. (Dep. Chem., Univ. Alberta, Edmonton, AB, Can.). J. Heterocycl. Chem., 30(5), 1181-9 (English) 1993. CODEN: JHTCAD. ISSN: 0022-152X.

GI

Searched by: Mary Hale 308-4258 CM-1 1E01



AB Alternative syntheses of (deoxy-.beta.-D-threo-pentofuranosyl)adenine I (R = OH, R1 = H) (II), the core nucleoside of agrocin 84 and its 2'-deoxy threo isomer I (R = H, R1 = OH) (III) were devised: (1) direct conversion of 9-(.beta.-D-arabinofuranosyl)adenine into 9-(2,3-anhydro-.beta.-D-lyxofuranosyl)adenine and regioselective opening of its oxirane ring with sodium borohydride to give II and III (.apprx.7.5:1); (2) treatment of adenosine with sodium hydride and 2,4,6-triisopropylbenzenesulfonyl chloride, and subjection of the resulting 2'(3')-sulfonates to the reductive [1,2]-hydride shift rearrangement with lithium triethylborohydride to give II and III (.apprx.2:1); and (3) subjection of the phenoxythiocarbonyl esters of 9-[2(3),5-bis-O-(tert-butyl)dimethylsilyl]-.beta.-D-arabinofuranosyl]adenine to Barton deoxygenation, and deprotection to give II and 2'-deoxyadenosine (.apprx.5:1). Methods (2) and (3) gave lower yields. Syntheses of simplified 6-N- and 5'-O-adenosine phosphoramidate model compds. were explored to examine potential access to such features in the structure proposed for agrocin 84.

L5 ANSWER 43 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 154534-47-1 REGISTRY

CN Phosphoramidic acid, (9-.beta.-D-ribofuranosyl-9H-purin-6-yl)-, diethyl ester (9CI) (CA INDEX NAME)

OTHER NAMES:

CN Adenosine 6-N-(O,O-diethylphosphoramidate)

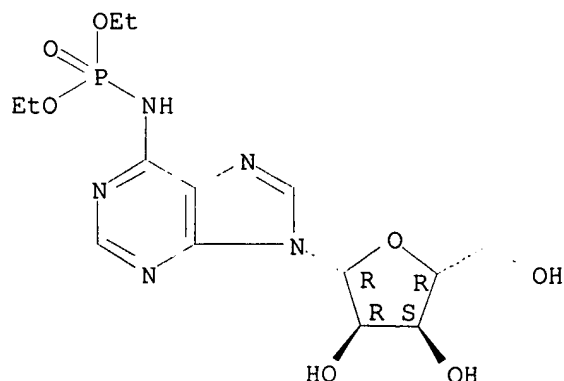
FS STEREOSEARCH

MF C14 H22 N5 O7 P

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

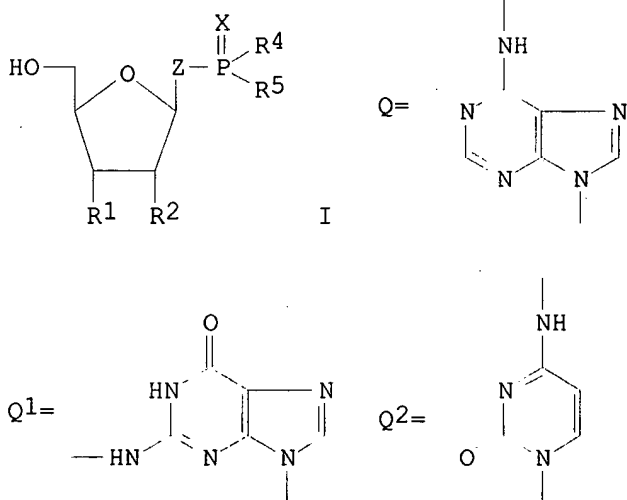


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 120:324143 Preparation of nucleic acid-related compounds.
Sekine, Mitsuo; Wada, Takeshi (Wako Pure Chem Ind Ltd, Japan). Jpn. Kokai
Tokkyo Koho JP 06009681 A2 19940118 Heisei, 11 pp. (Japanese). CODEN:
JKXXAF. APPLICATION: JP 1993-76085 19930310. PRIORITY: JP 1992-88134
19920312.

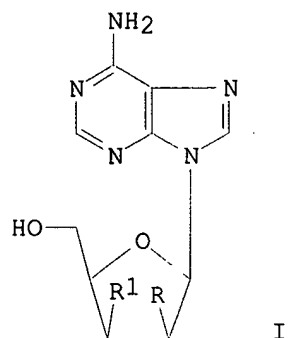
GI



AB Nucleoside N-(thio)phosphoramidate derivs. [I; R1, R2 = H, OH; Z = Q - Q2; X = O, S, Se; R4, R5 = OH, NH2, (un)substituted C1-18 alkoxy or aryloxy], useful as pharmaceuticals, agrochems., and medical diagnostic agents (no data), are prepd. Thus, 1,2,4-lH-triazole was dissolved in acetone and reacted with P(O)Cl3 and Et3N at 0.degree. for 30 min and then with a soln. of 2',3',5'-tri-O-benzoyladenosine in MeCN to give 80% triethylammonium 2',3',5'-tri-O-benzoyladenosine-6-N-(triazolyl)phosphoramidate, which was treated with concd. aq. NH3-pyridine mixt. to give, after purifn. by anion exchange chromatog. using DEA cellulose and lyophilization, 83% triethylammonium adenosine-6-N-(amino)phosphoramidate.

REFERENCE 2: 120:271041 Nucleic acid related compounds. 81. Syntheses of 9-(3-deoxy-.beta.-D-threo-pentofuranosyl)adenine, the core nucleoside of the extraordinarily selective antibiotic agrocin 84, and simplified structural component analogs. Vinayak, Ravi; Hansske, Fritz; Robins, Morris J. (Dep. Chem., Univ. Alberta, Edmonton, AB, Can.). J. Heterocycl. Chem., 30(5), 1181-9 (English) 1993. CODEN: JHTCAD. ISSN: 0022-152X.

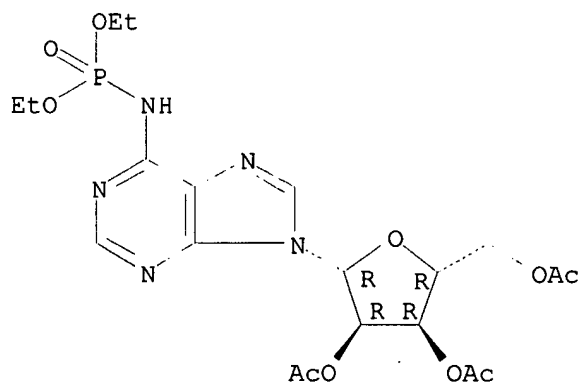
GI



AB Alternative syntheses of (deoxy-.beta.-D-threo-pentofuranosyl)adenine I (R = OH, R1 = H) (II), the core nucleoside of agrocin 84 and its 2'-deoxy threo isomer I (R = H, R1 = OH) (III) were devised: (1) direct conversion of 9-(.beta.-D-arabinofuranosyl)adenine into 9-(2,3-anhydro-.beta.-D-lyxofuranosyl)adenine and regioselective opening of its oxirane ring with sodium borohydride to give II and III (.apprx.7.5:1); (2) treatment of adenosine with sodium hydride and 2,4,6-triisopropylbenzenesulfonyl chloride, and subjection of the resulting 2'(3')-sulfonates to the reductive [1,2]-hydride shift rearrangement with lithium triethylborohydride to give II and III (.apprx.2:1); and (3) subjection of the phenoxythiocarbonyl esters of 9-[2(3),5-bis-O-(tert-butyl)dimethylsilyl]-.beta.-D-arabinofuranosyladenine to Barton deoxygenation, and deprotection to give II and 2'-deoxyadenosine (.apprx.5:1). Methods (2) and (3) gave lower yields. Syntheses of simplified 6-N- and 5'-O-adenosine phosphoramidate model compds. were explored to examine potential access to such features in the structure proposed for agrocin 84.

L5 ANSWER 44 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 154534-46-0 REGISTRY
 CN Phosphoramidic acid, [9-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, diethyl ester (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C20 H28 N5 O10 P
 CI COM
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.



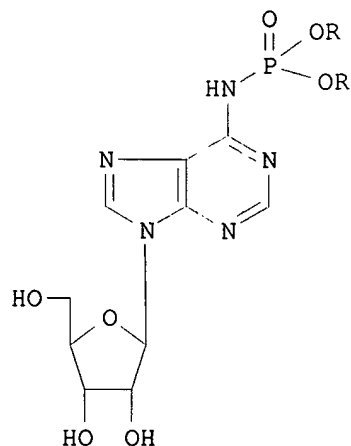
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1967 TO DATE)

3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 122:214406 Synthesis and Properties of N-Phosphorylated Ribonucleosides. Wada, Takeshi; Moriguchi, Tomohisa; Sekine, Mitsuo (Faculty of Bioscience and Biotechnology, Tokyo Institute of Technology, Yokohama, 227, Japan). J. Am. Chem. Soc., 116(22), 9901-11 (English) 1994. CODEN: JACSAT. ISSN: 0002-7863.

GI

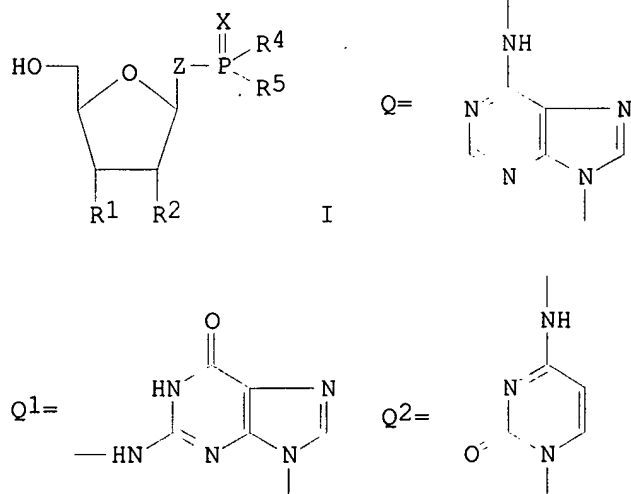


I

AB A new class of phosphorylated nucleosides,, e.g. I (R = Na, Et), were synthesized in good yields via phosphitylation of the amino group of appropriately protected adenosine derivs. In a similar manner, cytidine 4-N-phosphoramidate (4-N-CMP), guanosine 2-N-phosphoramidate (2-N-GMP), and their di-Et ester derivs. were synthesized. These new compds. were characterized by ¹H, ¹³C, and ³¹P NMR, UV, CD, IR, electrophoresis, and mass spectroscopy. The conformation and water soly. of these N-phosphorylated ribonucleoside derivs. have been studied in detail.

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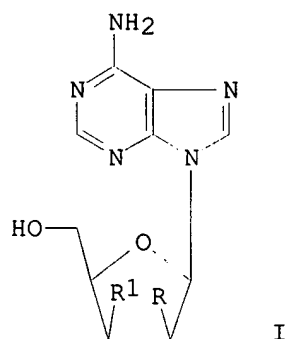
GI



AB Nucleoside N-(thio)phosphoramidate derivs. [I; R1, R2 = H, OH; Z = Q - Q2; X = O, S, Se; R4, R5 = OH, NH2, (un)substituted C1-18 alkoxy or aryloxy], useful as pharmaceuticals, agrochems., and medical diagnostic agents (no data), are prepd. Thus, 1,2,4-1H-triazole was dissolved in acetone and reacted with P(O)Cl3 and Et3N at 0.degree. for 30 min and then with a soln. of 2',3',5'-tri-O-benzoyladenosine in MeCN to give 80% triethylammonium 2',3',5'-tri-O-benzoyladenosine-6-N-(triazolyl)phosphoramidate, which was treated with concd. aq. NH3-pyridine mixt. to give, after purifn. by anion exchange chromatog. using DEA cellulose and lyophilization, 83% triethylammonium adenosine-6-N-(amino)phosphoramidate.

REFERENCE 3: 120:271041 Nucleic acid related compounds. 81. Syntheses of 9-(3-deoxy-.beta.-D-threo-pentofuranosyl)adenine, the core nucleoside of the extraordinarily selective antibiotic agrocin 84, and simplified structural component analogs. Vinayak, Ravi; Hansske, Fritz; Robins, Morris J. (Dep. Chem., Univ. Alberta, Edmonton, AB, Can.). J. Heterocycl. Chem., 30(5), 1181-9 (English) 1993. CODEN: JHTCAD. ISSN: 0022-152X.

GI

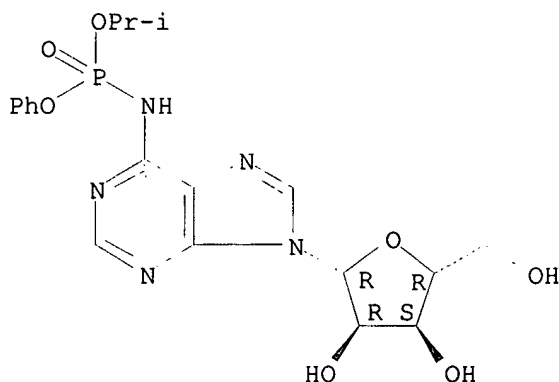


AB Alternative syntheses of (deoxy-.beta.-D-threo-pentofuranosyl)adenine I (R = OH, R1 = H) (II), the core nucleoside of agrocin 84 and its 2'-deoxy threo isomer I (R = H, R1 = OH) (III) were devised: (1) direct conversion of 9-(.beta.-D-arabinofuranosyl)adenine into 9-(2,3-anhydro-.beta.-D-

lyxofuranosyl)adenine and regioselective opening of its oxirane ring with sodium borohydride to give II and III (.apprx.7.5:1); (2) treatment of adenosine with sodium hydride and 2,4,6-triisopropylbenzenesulfonyl chloride, and subjection of the resulting 2'(3')-sulfonates to the reductive [1,2]-hydride shift rearrangement with lithium triethylborohydride to give II and III (.apprx.2:1); and (3) subjection of the phenoxythiocarbonyl esters of 9-[2(3),5-bis-O-(tert-butyldimethylsilyl)-.beta.-D-arabinofuranosyl]adenine to Barton deoxygenation, and deprotection to give II and 2'-deoxyadenosine (.apprx.5:1). Methods (2) and (3) gave lower yields. Syntheses of simplified 6-N- and 5'-O-adenosine phosphoramidate model compds. were explored to examine potential access to such features in the structure proposed for agrocin 84.

L5 ANSWER 45 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 154534-44-8 REGISTRY
 CN Phosphoramidic acid, (9-.beta.-D-ribofuranosyl-9H-purin-6-yl)-, 1-methylethyl phenyl ester (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C19 H24 N5 O7 P
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.

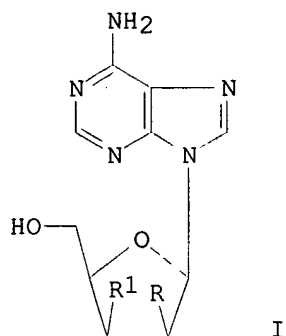


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 120:271041 Nucleic acid related compounds. 81. Syntheses of 9-(3-deoxy-.beta.-D-threo-pentofuranosyl)adenine, the core nucleoside of the extraordinarily selective antibiotic agrocin 84, and simplified structural component analogs. Vinayak, Ravi; Hansske, Fritz; Robins, Morris J. (Dep. Chem., Univ. Alberta, Edmonton, AB, Can.). J. Heterocycl. Chem., 30(5), 1181-9 (English) 1993. CODEN: JHTCAD. ISSN: 0022-152X.

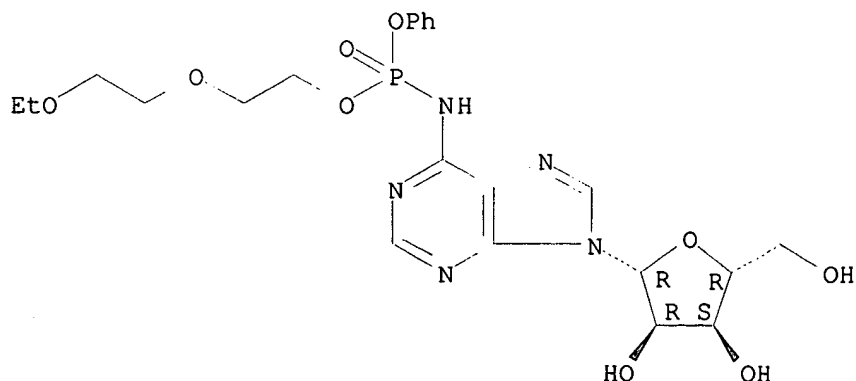
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AB Alternative syntheses of (deoxy-.beta.-D-threo-pentofuranosyl)adenine I (R = OH, R1 = H) (II), the core nucleoside of agrocin 84 and its 2'-deoxy threo isomer I (R = H, R1 = OH) (III) were devised: (1) direct conversion of 9-(.beta.-D-arabinofuranosyl)adenine into 9-(2,3-anhydro-.beta.-D-lyxofuranosyl)adenine and regioselective opening of its oxirane ring with sodium borohydride to give II and III (.apprx.7.5:1); (2) treatment of adenosine with sodium hydride and 2,4,6-triisopropylbenzenesulfonyl chloride, and subjection of the resulting 2'(3')-sulfonates to the reductive [1,2]-hydride shift rearrangement with lithium triethylborohydride to give II and III (.apprx.2:1); and (3) subjection of the phenoxythiocarbonyl esters of 9-[2(3),5-bis-O-(tert-butylidimethylsilyl)-.beta.-D-arabinofuranosyl]adenine to Barton deoxygenation, and deprotection to give II and 2'-deoxyadenosine (.apprx.5:1). Methods (2) and (3) gave lower yields. Syntheses of simplified 6-N- and 5'-O-adenosine phosphoramidate model compds. were explored to examine potential access to such features in the structure proposed for agrocin 84.

L5 ANSWER 46 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 154534-43-7 REGISTRY
 CN Phosphoramidic acid, (9-.beta.-D-ribofuranosyl-9H-purin-6-yl)-, 2-(2-ethoxyethoxy)ethyl phenyl ester (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C22 H30 N5 O9 P
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.



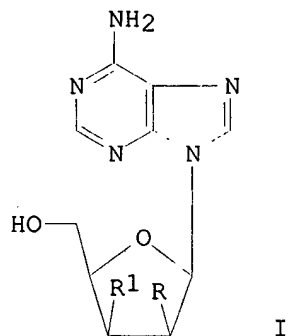
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 120:271041 Nucleic acid related compounds. 81. Syntheses of 9-(3-deoxy-.beta.-D-threo-pentofuranosyl)adenine, the core nucleoside of the extraordinarily selective antibiotic agrocin 84, and simplified structural component analogs. Vinayak, Ravi; Hansske, Fritz; Robins, Morris J. (Dep. Chem., Univ. Alberta, Edmonton, AB, Can.). J. Heterocycl. Chem., 30(5), 1181-9 (English) 1993. CODEN: JHTCAD. ISSN: 0022-152X.

GI



AB Alternative syntheses of (deoxy-.beta.-D-threo-pentofuranosyl)adenine I (R = OH, R1 = H) (II), the core nucleoside of agrocin 84 and its 2'-deoxy threo isomer I (R = H, R1 = OH) (III) were devised: (1) direct conversion of 9-(.beta.-D-arabinofuranosyl)adenine into 9-(2,3-anhydro-.beta.-D-lyxofuranosyl)adenine and regioselective opening of its oxirane ring with sodium borohydride to give II and III (.apprx.7.5:1); (2) treatment of adenosine with sodium hydride and 2,4,6-triisopropylbenzenesulfonyl chloride, and subjection of the resulting 2'(3')-sulfonates to the reductive [1,2]-hydride shift rearrangement with lithium triethylborohydride to give II and III (.apprx.2:1); and (3) subjection of the phenoxythiocarbonyl esters of 9-[2(3),5-bis-O-(tert-butyl)dimethylsilyl]-.beta.-D-arabinofuranosyladenine to Barton deoxygenation, and deprotection to give II and 2'-deoxyadenosine (.apprx.5:1). Methods (2) and (3) gave lower yields. Syntheses of simplified 6-N- and 5'-O-adenosine phosphoramidate model compds. were explored to examine potential access to such features in the structure proposed for agrocin 84.

L5 ANSWER 47 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 154534-42-6 REGISTRY

CN Phosphoramidic acid, (9-.beta.-D-ribofuranosyl-9H-purin-6-yl)-, ethyl phenyl ester (9CI) (CA INDEX NAME)

FS STEREOSEARCH

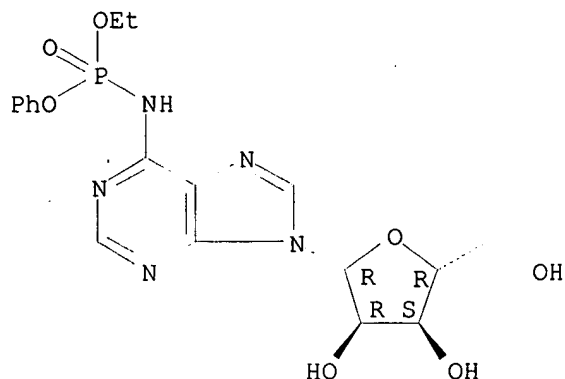
MF C18 H22 N5 O7 P

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Searched by: Mary Hale 308-4258 CM-1 1E01

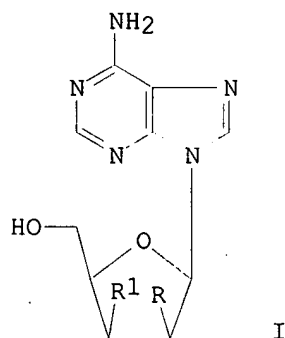


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 120:271041 Nucleic acid related compounds. 81. Syntheses of 9-(3-deoxy-.beta.-D-threo-pentofuranosyl)adenine, the core nucleoside of the extraordinarily selective antibiotic agrocin 84, and simplified structural component analogs. Vinayak, Ravi; Hansske, Fritz; Robins, Morris J. (Dep. Chem., Univ. Alberta, Edmonton, AB, Can.). J. Heterocycl. Chem., 30(5), 1181-9 (English) 1993. CODEN: JHTCAD. ISSN: 0022-152X.

GI

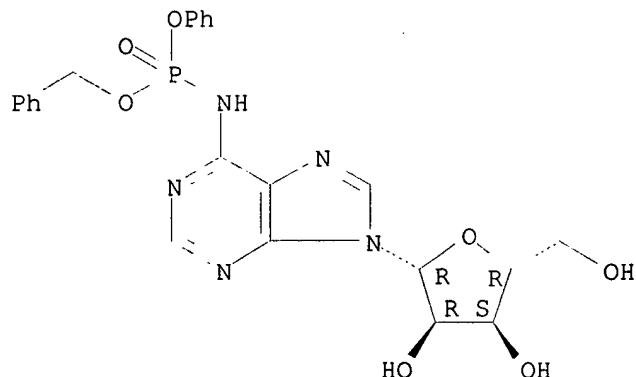


AB Alternative syntheses of (deoxy-.beta.-D-threo-pentofuranosyl)adenine I (R = OH, R1 = H) (II), the core nucleoside of agrocin 84 and its 2'-deoxy threo isomer I (R = H, R1 = OH) (III) were devised: (1) direct conversion of 9-(.beta.-D-arabinofuranosyl)adenine into 9-(2,3-anhydro-.beta.-D-lyxofuranosyl)adenine and regioselective opening of its oxirane ring with sodium borohydride to give II and III (.apprx.7.5:1); (2) treatment of adenosine with sodium hydride and 2,4,6-triisopropylbenzenesulfonyl chloride, and subjection of the resulting 2'(3')-sulfonates to the reductive [1,2]-hydride shift rearrangement with lithium triethylborohydride to give II and III (.apprx.2:1); and (3) subjection of the phenoxythiocarbonyl esters of 9-[2(3),5-bis-O-(tert-butyltrimethylsilyl)-.beta.-D-arabinofuranosyl]adenine to Barton deoxygenation, and deprotection to give II and 2'-deoxyadenosine (.apprx.5:1). Methods (2) and (3) gave lower yields. Syntheses of simplified 6-N- and 5'-O-adenosine phosphoramidate model compds. were

explored to examine potential access to such features in the structure proposed for agrocin 84.

L5 ANSWER 48 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 154534-41-5 REGISTRY
CN Phosphoramidic acid, (9-.beta.-D-ribofuranosyl-9H-purin-6-yl)-, phenyl phenylmethyl ester (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C23 H24 N5 O7 P
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

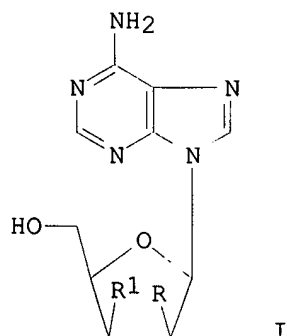


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 120:271041 Nucleic acid related compounds. 81. Syntheses of 9-(3-deoxy-.beta.-D-threo-pentofuranosyl)adenine, the core nucleoside of the extraordinarily selective antibiotic agrocin 84, and simplified structural component analogs. Vinayak, Ravi; Hansske, Fritz; Robins, Morris J. (Dep. Chem., Univ. Alberta, Edmonton, AB, Can.). J. Heterocycl. Chem., 30(5), 1181-9 (English) 1993. CODEN: JHTCAD. ISSN: 0022-152X.

GI



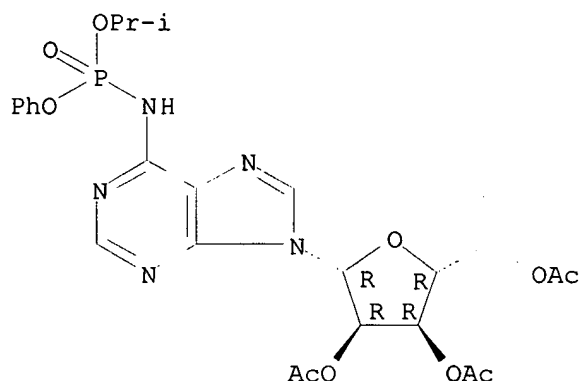
AB Alternative syntheses of (deoxy-.beta.-D-threo-pentofuranosyl)adenine I (R = OH, R1 = H) (II), the core nucleoside of agrocin 84 and its 2'-deoxy

Searched by: Mary Hale 308-4258 CM-1 1E01

threo isomer I (R = H, R1 = OH) (III) were devised: (1) direct conversion of 9-(.beta.-D-arabinofuranosyl)adenine into 9-(2,3-anhydro-.beta.-D-lyxofuranosyl)adenine and regioselective opening of its oxirane ring with sodium borohydride to give II and III (.apprx.7.5:1); (2) treatment of adenosine with sodium hydride and 2,4,6-triisopropylbenzenesulfonyl chloride, and subjection of the resulting 2'(3')-sulfonates to the reductive [1,2]-hydride shift rearrangement with lithium triethylborohydride to give II and III (.apprx.2:1); and (3) subjection of the phenoxythiocarbonyl esters of 9-[2(3),5-bis-O-(tert-butyldimethylsilyl)-.beta.-D-arabinofuranosyl]adenine to Barton deoxygenation, and deprotection to give II and 2'-deoxyadenosine (.apprx.5:1). Methods (2) and (3) gave lower yields. Syntheses of simplified 6-N- and 5'-O-adenosine phosphoramidate model compds. were explored to examine potential access to such features in the structure proposed for agrocin 84.

L5 ANSWER 49 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 154534-40-4 REGISTRY
 CN Phosphoramidic acid, [9-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, 1-methylethyl phenyl ester (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C25 H30 N5 O10 P
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.

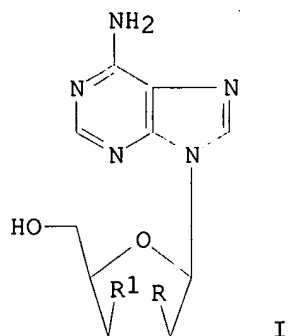


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 120:271041 Nucleic acid related compounds. 81. Syntheses of 9-(3-deoxy-.beta.-D-threo-pentofuranosyl)adenine, the core nucleoside of the extraordinarily selective antibiotic agrocin 84, and simplified structural component analogs. Vinayak, Ravi; Hansske, Fritz; Robins, Morris J. (Dep. Chem., Univ. Alberta, Edmonton, AB, Can.). J. Heterocycl. Chem., 30(5), 1181-9 (English) 1993. CODEN: JHTCAD. ISSN: 0022-152X.

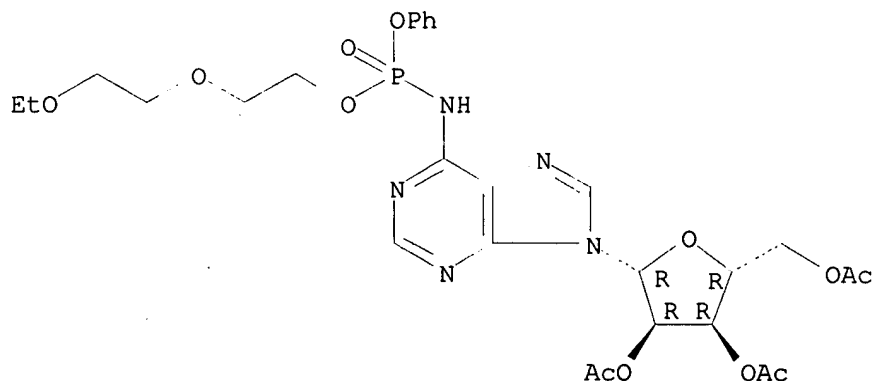
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AB Alternative syntheses of (deoxy-.beta.-D-threo-pentofuranosyl)adenine I (R = OH, R1 = H) (II), the core nucleoside of agrocin 84 and its 2'-deoxy threo isomer I (R = H, R1 = OH) (III) were devised: (1) direct conversion of 9-(.beta.-D-arabinofuranosyl)adenine into 9-(2,3-anhydro-.beta.-D-lyxofuranosyl)adenine and regioselective opening of its oxirane ring with sodium borohydride to give II and III (.apprx.7.5:1); (2) treatment of adenosine with sodium hydride and 2,4,6-triisopropylbenzenesulfonyl chloride, and subjection of the resulting 2'(3')-sulfonates to the reductive [1,2]-hydride shift rearrangement with lithium triethylborohydride to give II and III (.apprx.2:1); and (3) subjection of the phenoxythiocarbonyl esters of 9-[2(3),5-bis-O-(tert-butyltrimethylsilyl)-.beta.-D-arabinofuranosyl]adenine to Barton deoxygenation, and deprotection to give II and 2'-deoxyadenosine (.apprx.5:1). Methods (2) and (3) gave lower yields. Syntheses of simplified 6-N- and 5'-O-adenosine phosphoramidate model compds. were explored to examine potential access to such features in the structure proposed for agrocin 84.

L5 ANSWER 50 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 154534-39-1 REGISTRY
 CN Phosphoramidic acid, [9-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, 2-(2-ethoxyethoxy)ethyl phenyl ester (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C28 H36 N5 O12 P
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.



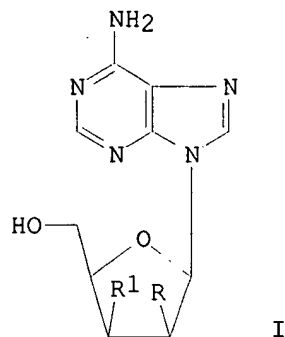
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 120:271041 Nucleic acid related compounds. 81. Syntheses of 9-(3-deoxy-.beta.-D-threo-pentofuranosyl)adenine, the core nucleoside of the extraordinarily selective antibiotic agrocin 84, and simplified structural component analogs. Vinayak, Ravi; Hansske, Fritz; Robins, Morris J. (Dep. Chem., Univ. Alberta, Edmonton, AB, Can.). J. Heterocycl. Chem., 30(5), 1181-9 (English) 1993. CODEN: JHTCAD. ISSN: 0022-152X.

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AB Alternative syntheses of (deoxy-.beta.-D-threo-pentofuranosyl)adenine I (R = OH, R1 = H) (II), the core nucleoside of agrocin 84 and its 2'-deoxy threo isomer I (R = H, R1 = OH) (III) were devised: (1) direct conversion of 9-(.beta.-D-arabinofuranosyl)adenine into 9-(2,3-anhydro-.beta.-D-lyxofuranosyl)adenine and regioselective opening of its oxirane ring with sodium borohydride to give II and III (.apprx.7.5:1); (2) treatment of adenosine with sodium hydride and 2,4,6-triisopropylbenzenesulfonyl chloride, and subjection of the resulting 2'(3')-sulfonates to the reductive [1,2]-hydride shift rearrangement with lithium triethylborohydride to give II and III (.apprx.2:1); and (3) subjection of the phenoxythiocarbonyl esters of 9-[2(3),5-bis-O-(tert-butyl)dimethylsilyl]-.beta.-D-arabinofuranosyl]adenine to Barton deoxygenation, and deprotection to give II and 2'-deoxyadenosine (.apprx.5:1). Methods (2) and (3) gave lower yields. Syntheses of simplified 6-N- and 5'-O-adenosine phosphoramidate model compds. were explored to examine potential access to such features in the structure proposed for agrocin 84.

L5 ANSWER 51 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 154534-38-0 REGISTRY

CN Phosphoramidic acid, [9-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, ethyl phenyl ester (9CI) (CA INDEX NAME)

FS STEREOSEARCH

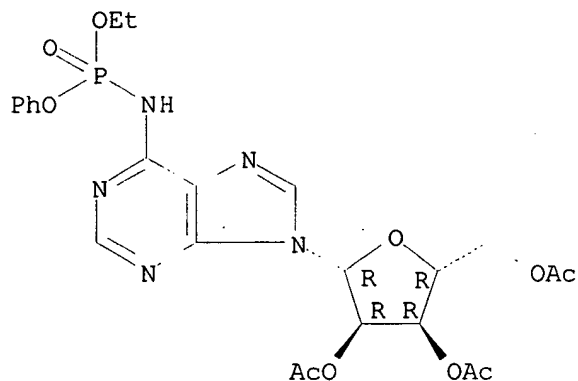
MF C24 H28 N5 O10 P

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Searched by: Mary Hale 308-4258 CM-1 1E01

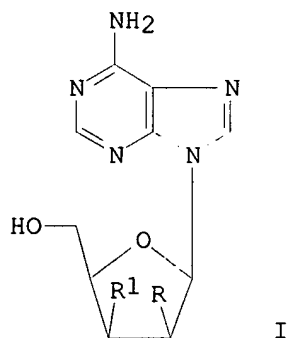


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 120:271041 Nucleic acid related compounds. 81. Syntheses of 9-(3-deoxy-.beta.-D-threo-pentofuranosyl)adenine, the core nucleoside of the extraordinarily selective antibiotic agrocin 84, and simplified structural component analogs. Vinayak, Ravi; Hansske, Fritz; Robins, Morris J. (Dep. Chem., Univ. Alberta, Edmonton, AB, Can.). J. Heterocycl. Chem., 30(5), 1181-9 (English) 1993. CODEN: JHTCAD. ISSN: 0022-152X.

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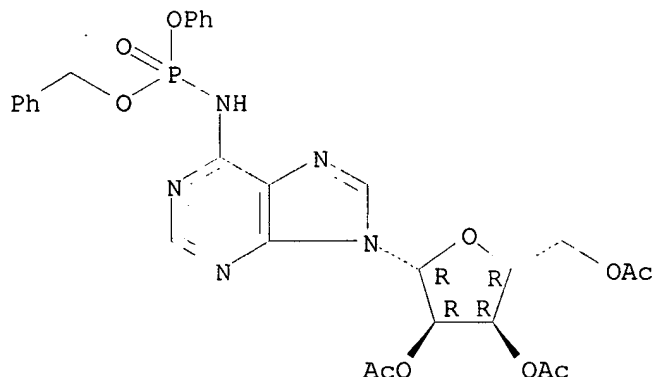


AB Alternative syntheses of (deoxy-.beta.-D-threo-pentofuranosyl)adenine I (R = OH, R1 = H) (II), the core nucleoside of agrocin 84 and its 2'-deoxy threo isomer I (R = H, R1 = OH) (III) were devised: (1) direct conversion of 9-(.beta.-D-arabinofuranosyl)adenine into 9-(2,3-anhydro-.beta.-D-lyxofuranosyl)adenine and regioselective opening of its oxirane ring with sodium borohydride to give II and III (.apprx.7.5:1); (2) treatment of adenosine with sodium hydride and 2,4,6-triisopropylbenzenesulfonyl chloride, and subjection of the resulting 2'(3')-sulfonates to the reductive [1,2]-hydride shift rearrangement with lithium triethylborohydride to give II and III (.apprx.2:1); and (3) subjection of the phenoxythiocarbonyl esters of 9-[2(3),5-bis-O-(tert-butyltrimethylsilyl)-.beta.-D-arabinofuranosyl]adenine to Barton deoxygenation, and deprotection to give II and 2'-deoxyadenosine (.apprx.5:1). Methods (2) and (3) gave lower yields. Syntheses of simplified 6-N- and 5'-O-adenosine phosphoramidate model compds. were

explored to examine potential access to such features in the structure proposed for agrocin 84.

L5 ANSWER 52 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 154534-37-9 REGISTRY
CN Phosphoramidic acid, [9-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, phenyl phenylmethyl ester (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C29 H30 N5 O10 P
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

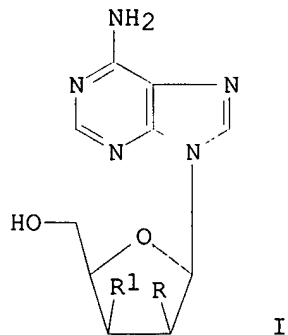


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 120:271041 Nucleic acid related compounds. 81. Syntheses of 9-(3-deoxy-.beta.-D-threo-pentofuranosyl)adenine, the core nucleoside of the extraordinarily selective antibiotic agrocin 84, and simplified structural component analogs. Vinayak, Ravi; Hansske, Fritz; Robins, Morris J. (Dep. Chem., Univ. Alberta, Edmonton, AB, Can.). J. Heterocycl. Chem., 30(5), 1181-9 (English) 1993. CODEN: JHTCAD. ISSN: 0022-152X.

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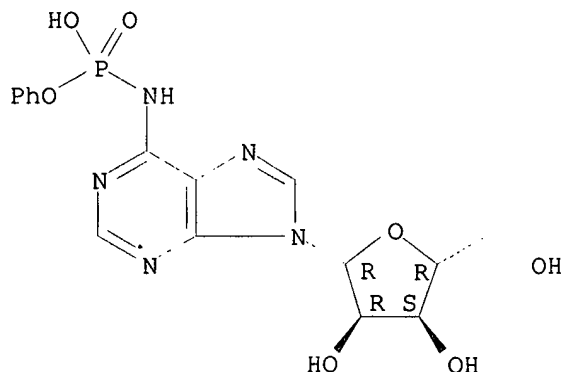
AB Alternative syntheses of (deoxy-.beta.-D-threo-pentofuranosyl)adenine I (R = OH, R1 = H) (II), the core nucleoside of agrocin 84 and its 2'-deoxy

Searched by: Mary Hale 308-4258 CM-1 1E01

threo isomer I (R = H, R1 = OH) (III) were devised: (1) direct conversion of 9-(.beta.-D-arabinofuranosyl)adenine into 9-(2,3-anhydro-.beta.-D-lyxofuranosyl)adenine and regioselective opening of its oxirane ring with sodium borohydride to give II and III (.apprx.7.5:1); (2) treatment of adenosine with sodium hydride and 2,4,6-triisopropylbenzenesulfonyl chloride, and subjection of the resulting 2'(3')-sulfonates to the reductive [1,2]-hydride shift rearrangement with lithium triethylborohydride to give II and III (.apprx.2:1); and (3) subjection of the phenoxythiocarbonyl esters of 9-[2(3),5-bis-O-(tert-butyltrimethylsilyl)-.beta.-D-arabinofuranosyl]adenine to Barton deoxygenation, and deprotection to give II and 2'-deoxyadenosine (.apprx.5:1). Methods (2) and (3) gave lower yields. Syntheses of simplified 6-N- and 5'-O-adenosine phosphoramidate model compds. were explored to examine potential access to such features in the structure proposed for agrocin 84.

L5 ANSWER 53 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 154534-36-8 REGISTRY
 CN Phosphoramidic acid, (9-.beta.-D-ribofuranosyl-9H-purin-6-yl)-, monophenyl ester (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C16 H18 N5 O7 P
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.



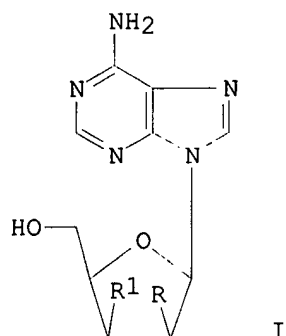
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 120:271041 Nucleic acid related compounds. 81. Syntheses of 9-(3-deoxy-.beta.-D-threo-pentofuranosyl)adenine, the core nucleoside of the extraordinarily selective antibiotic agrocin 84, and simplified structural component analogs. Vinayak, Ravi; Hansske, Fritz; Robins, Morris J. (Dep. Chem., Univ. Alberta, Edmonton, AB, Can.). J. Heterocycl. Chem., 30(5), 1181-9 (English) 1993. CODEN: JHTCAD. ISSN: 0022-152X.

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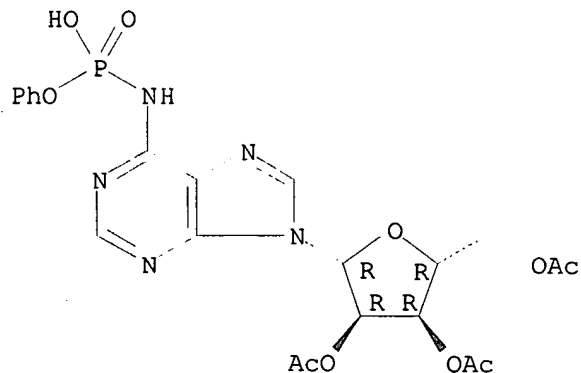
Searched by: Mary Hale 308-4258 CM-1 1E01



AB Alternative syntheses of (deoxy-.beta.-D-threo-pentofuranosyl)adenine I (R = OH, R1 = H) (II), the core nucleoside of agrocin 84 and its 2'-deoxy threo isomer I (R = H, R1 = OH) (III) were devised: (1) direct conversion of 9-(.beta.-D-arabinofuranosyl)adenine into 9-(2,3-anhydro-.beta.-D-lyxofuranosyl)adenine and regioselective opening of its oxirane ring with sodium borohydride to give II and III (.apprx.7.5:1); (2) treatment of adenosine with sodium hydride and 2,4,6-triisopropylbenzenesulfonyl chloride, and subjection of the resulting 2'(3')-sulfonates to the reductive [1,2]-hydride shift rearrangement with lithium triethylborohydride to give II and III (.apprx.2:1); and (3) subjection of the phenoxythiocarbonyl esters of 9-[2(3),5-bis-O-(tert-butylidimethylsilyl)-.beta.-D-arabinofuranosyl]adenine to Barton deoxygenation, and deprotection to give II and 2'-deoxyadenosine (.apprx.5:1). Methods (2) and (3) gave lower yields. Syntheses of simplified 6-N- and 5'-O-adenosine phosphoramidate model compds. were explored to examine potential access to such features in the structure proposed for agrocin 84.

L5 ANSWER 54 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 154534-35-7 REGISTRY
 CN Phosphoramidic acid, [9-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, monophenyl ester (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C22 H24 N5 O10 P
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.



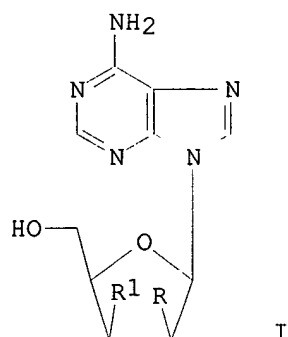
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

Searched by: Mary Hale 308-4258 CM-1 1E01

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 120:271041 Nucleic acid related compounds. 81. Syntheses of 9-(3-deoxy-.beta.-D-threo-pentofuranosyl)adenine, the core nucleoside of the extraordinarily selective antibiotic agrocin 84, and simplified structural component analogs. Vinayak, Ravi; Hansske, Fritz; Robins, Morris J. (Dep. Chem., Univ. Alberta, Edmonton, AB, Can.). J. Heterocycl. Chem., 30(5), 1181-9 (English) 1993. CODEN: JHTCAD. ISSN: 0022-152X.

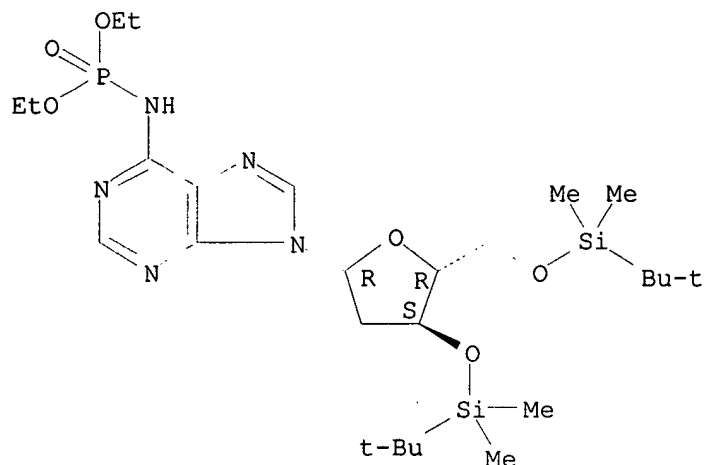
GI



AB Alternative syntheses of (deoxy-.beta.-D-threo-pentofuranosyl)adenine I (R = OH, R1 = H) (II), the core nucleoside of agrocin 84 and its 2'-deoxy threo isomer I (R = H, R1 = OH) (III) were devised: (1) direct conversion of 9-(.beta.-D-arabinofuranosyl)adenine into 9-(2,3-anhydro-.beta.-D-lyxofuranosyl)adenine and regioselective opening of its oxirane ring with sodium borohydride to give II and III (.apprx.7.5:1); (2) treatment of adenosine with sodium hydride and 2,4,6-triisopropylbenzenesulfonyl chloride, and subjection of the resulting 2'(3')-sulfonates to the reductive [1,2]-hydride shift rearrangement with lithium triethylborohydride to give II and III (.apprx.2:1); and (3) subjection of the phenoxythiocarbonyl esters of 9-[2(3),5-bis-O-(tert-butyl)dimethylsilyl]-.beta.-D-arabinofuranosyl]adenine to Barton deoxygenation, and deprotection to give II and 2'-deoxyadenosine (.apprx.5:1). Methods (2) and (3) gave lower yields. Syntheses of simplified 6-N- and 5'-O-adenosine phosphoramidate model compds. were explored to examine potential access to such features in the structure proposed for agrocin 84.

L5 ANSWER 55 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 145550-43-2 REGISTRY
CN Phosphoramidic acid, [[2-deoxy-3,5-bis-O-[(1,1-dimethylethyl)dimethylsilyl]-.beta.-D-erythro-pentofuranosyl]-9H-purin-6-yl]-, diethyl ester (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C26 H50 N5 O6 P Si2
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 118:81317 O-selective phosphorylation of nucleosides without N-protection. Uchiyama, Mamoru; Aso, Yoshio; Noyori, Ryoji; Hayakawa, Yoshihiro (Fac. Sci., Nagoya Univ., Nagoya, 464-01, Japan). J. Org. Chem., 58(2), 373-9 (English) 1993. CODEN: JOCEAH. ISSN: 0022-3263.

AB A facile chemoselective O-phosphorylation of N-unprotected nucleosides has been achieved via metal alkoxide formation. Sequential treatment of N-unprotected nucleosides with an equimolar amt. of an organometallic base, such as an alkyllithium, Me₃COK, Me₃CMgCl, LiAl(NMe₂)₄, Al(NMe₂)₃, (Me₂CHCH₂)₂AlH, etc., and a phosphorochloridate or p-nitrophenyl phosphate results in rapid O-phosphorylation to give the nucleotides in high yield. The method using magnesium alkoxides is the best in chemoselectivity, generality, and operational simplicity. The origin of the obsd. chemoselectivity is discussed.

L5 ANSWER 56 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 145550-40-9 REGISTRY

CN Phosphoramidic acid, [[2-deoxy-5-O-[(1,1-dimethylethyl)dimethylsilyl]-.beta.-D-erythro-pentofuranosyl]-9H-purin-6-yl]-, bis(2-chlorophenyl) ester (9CI) (CA INDEX NAME)

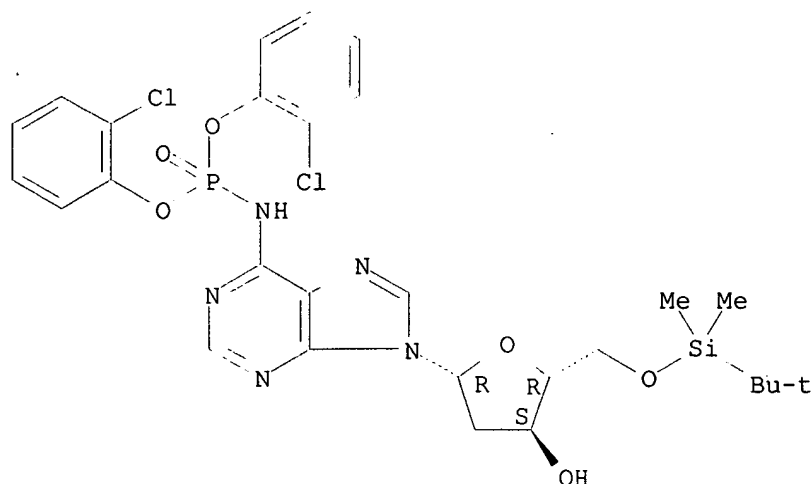
FS STEREOSEARCH

MF C28 H34 Cl2 N5 O6 P Si

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

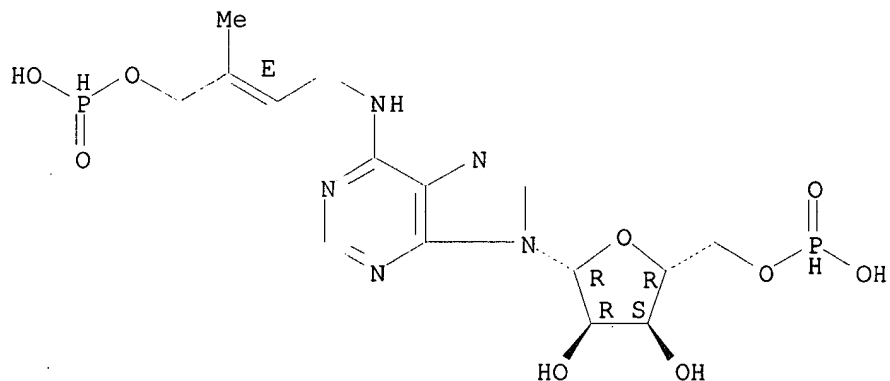
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 118:81317 O-selective phosphorylation of nucleosides without N-protection. Uchiyama, Mamoru; Aso, Yoshio; Noyori, Ryoji; Hayakawa, Yoshihiro (Fac. Sci., Nagoya Univ., Nagoya, 464-01, Japan). J. Org. Chem., 58(2), 373-9 (English) 1993. CODEN: JOCEAH. ISSN: 0022-3263.

AB A facile chemoselective O-phosphorylation of N-unprotected nucleosides has been achieved via metal alkoxide formation. Sequential treatment of N-unprotected nucleosides with an equimolar amt. of an organometallic base, such as an alkyllithium, Me₃COK, Me₃CMgCl, LiAl(NMe₂)₄, Al(NMe₂)₃, (Me₂CHCH₂)₂AlH, etc., and a phosphorochloridate or p-nitrophenyl phosphate results in rapid O-phosphorylation to give the nucleotides in high yield. The method using magnesium alkoxides is the best in chemoselectivity, generality, and operational simplicity. The origin of the obsd. chemoselectivity is discussed.

L5 ANSWER 57 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 129789-00-0 REGISTRY
CN Adenosine, N-[4-[(hydroxyphosphinyl)oxy]-3-methyl-2-butenyl]-, 5'-(hydrogen phosphonate), (E)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C15 H23 N5 O9 P2
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

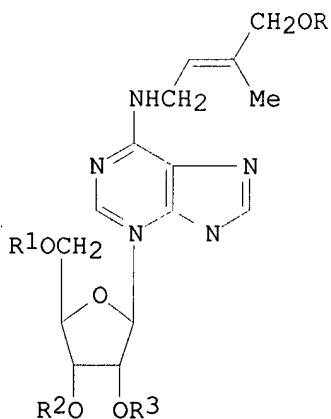
Absolute stereochemistry.
Double bond geometry as shown.



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 113:172616 The synthesis of phosphorus derivatives of ribosyl zeatin. Shadid, Belal; Van der Plas, Henk C. (Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.). Tetrahedron, 46(6), 2179-86 (English) 1990. CODEN: TETRAB. ISSN: 0040-4020.

GI



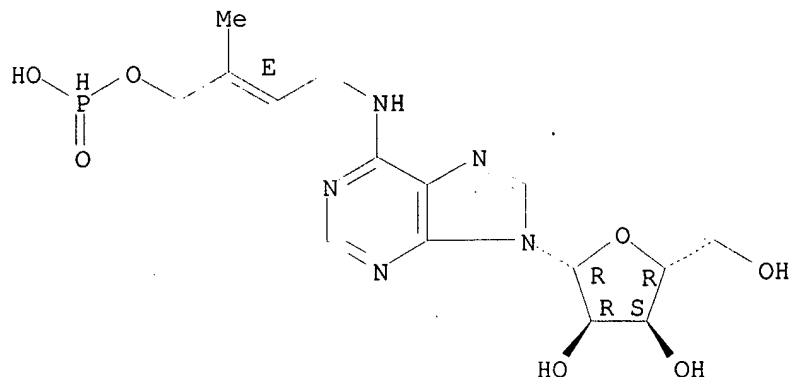
I

AB Sulfur was used for the conversion of ribosyl zeatin phosphonate I [R = PH(O)OH, R1 = SiMe2CMe3, PH(O)OH, R2R3 = CHOMe] (II) into the corresponding thiophosphates I [R = P(S)(OH)2]. 2,2'-Dipyridyldisulfide in the presence of MeOH was used for the conversion of II into the corresponding Me phosphates I [R = P(O)(OH)OMe]. Deprotection of these compds. gave the phosphorus derivs. of ribosyl zeatin I [R, R1 = H, PH(O)OH, P(O)(OH)OMe, P(S)(OH)2; R2 = R3 = H].

L5 ANSWER 58 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 129788-99-4 REGISTRY
CN Adenosine, N-[4-[(hydroxyphosphinyl)oxy]-3-methyl-2-butenyl]-, (E)- (9CI)
(CA INDEX NAME)
FS STEREOSEARCH
MF C15 H22 N5 O7 P
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Searched by: Mary Hale 308-4258 CM-1 1E01

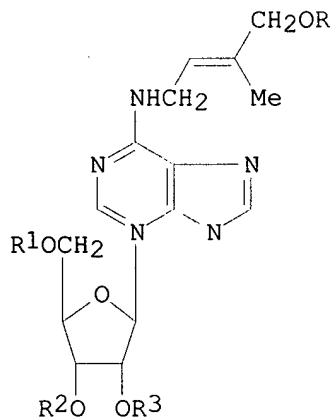
Absolute stereochemistry.
Double bond geometry as shown.



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 113:172616 The synthesis of phosphorus derivatives of ribosyl zeatin. Shadid, Belal; Van der Plas, Henk C. (Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.). Tetrahedron, 46(6), 2179-86 (English) 1990. CODEN: TETRAB. ISSN: 0040-4020.

GI



I

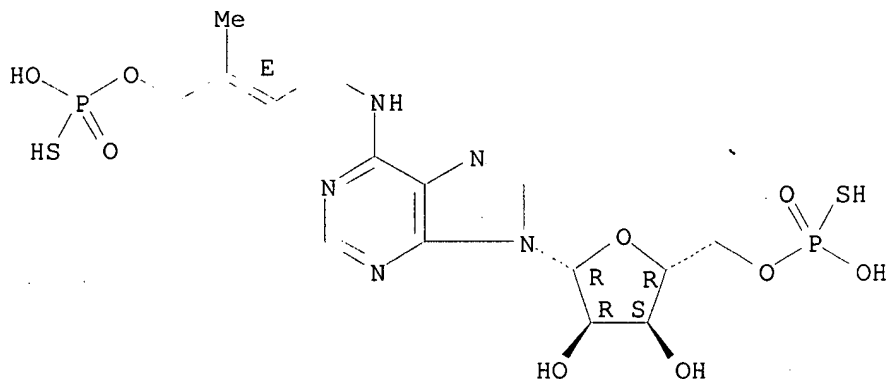
AB Sulfur was used for the conversion of ribosyl zeatin phosphonate I [R = PH(O)OH, R1 = SiMe2CMe3, PH(O)OH, R2R3 = CHOMe] (II) into the corresponding thiophosphates I [R = P(S)(OH)2]. 2,2'-Dipyridyldisulfide in the presence of MeOH was used for the conversion of II into the corresponding Me phosphates I [R = P(O)(OH)OMe]. Deprotection of these compds. gave the phosphorus derivs. of ribosyl zeatin I [R, R1 = H, PH(O)OH, P(O)(OH)OMe, P(S)(OH)2; R2 = R3 = H].

L5 ANSWER 59 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 129788-98-3 REGISTRY
CN Adenosine, N-[4-[(hydroxymercaptoposphinyl)oxy]-3-methyl-2-butenyl]-, 5'-(dihydrogen phosphorothioate), (E)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C15 H23 N5 O9 P2 S2

Searched by: Mary Hale 308-4258 CM-1 1E01

SR CA
 LC STN Files: BEILSTEIN*, CA, CAPLUS
 (*File contains numerically searchable property data)

Absolute stereochemistry.
 Double bond geometry as shown.

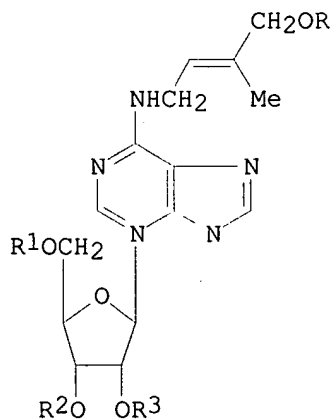


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 113:172616 The synthesis of phosphorus derivatives of ribosyl zeatin. Shadid, Belal; Van der Plas, Henk C. (Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.). Tetrahedron, 46(6), 2179-86 (English) 1990. CODEN: TETRAB. ISSN: 0040-4020.

GI



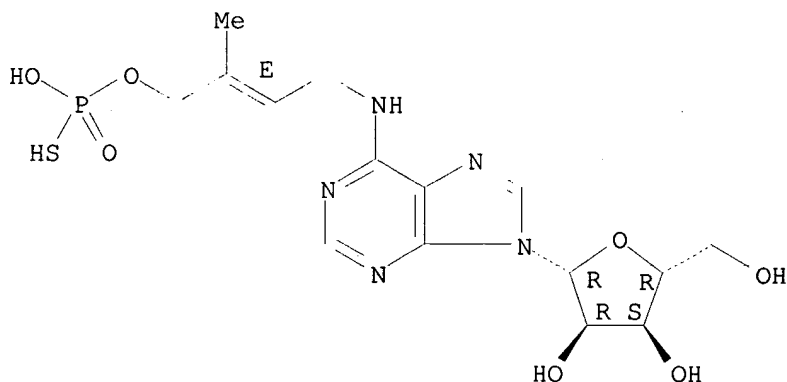
I

AB Sulfur was used for the conversion of ribosyl zeatin phosphonate I [R = PH(O)OH, R1 = SiMe2CMe3, PH(O)OH, R2R3 = CHOMe] (II) into the corresponding thiophosphates I [R = P(S)(OH)2]. 2,2'-Dipyridyldisulfide in the presence of MeOH was used for the conversion of II into the corresponding Me phosphates I [R = P(O)(OH)OMe]. Deprotection of these compds. gave the phosphorus derivs. of ribosyl zeatin I [R, R1 = H, PH(O)OH, P(O)(OH)OMe, P(S)(OH)2; R2 = R3 = H].

Searched by: Mary Hale 308-4258 CM-1 1E01

L5 ANSWER 60 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 129788-97-2 REGISTRY
 CN Adenosine, N-[4-[(hydroxymercaptophosphinyl)oxy]-3-methyl-2-butenyl]-, (E)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C15 H22 N5 O7 P S
 SR CA
 LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.
 Double bond geometry as shown.

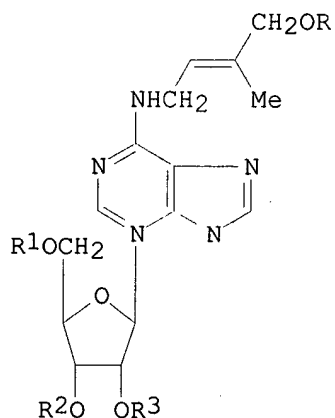


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 113:172616 The synthesis of phosphorus derivatives of ribosyl zeatin. Shadid, Belal; Van der Plas, Henk C. (Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.). Tetrahedron, 46(6), 2179-86 (English) 1990. CODEN: TETRAB. ISSN: 0040-4020.

GI



I

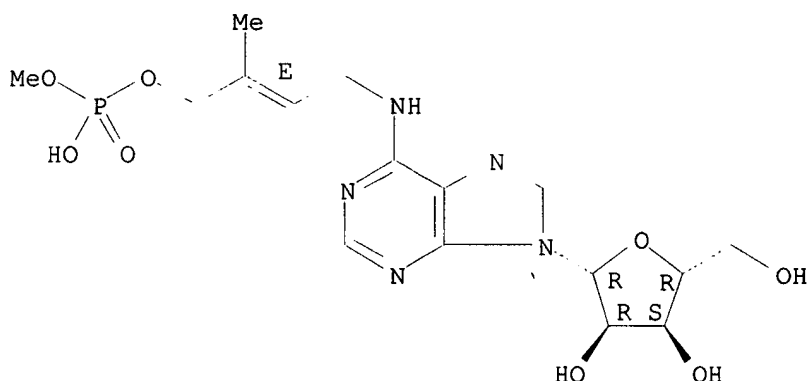
AB Sulfur was used for the conversion of ribosyl zeatin phosphonate I [R = PH(O)OH, R1 = SiMe2CMe3, PH(O)OH, R2R3 = CHOMe] (II) into the corresponding thiophosphates I [R=P(S)(OH)2]. 2,2'-Dipyridyldisulfide in

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the presence of MeOH was used for the conversion of II into the corresponding Me phosphates I [R = P(O)(OH)OMe]. Deprotection of these compds. gave the phosphorus derivs. of ribosyl zeatin I [R, R1 = H, PH(O)OH, P(O)(OH)OMe, P(S)(OH)2; R2 = R3 = H].

L5 ANSWER 61 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 129788-96-1 REGISTRY
CN Adenosine, N-[4-[(hydroxymethoxyphosphinyl)oxy]-3-methyl-2-butenyl]-, (E)-
(9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C16 H24 N5 O8 P
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)

Absolute stereochemistry.
Double bond geometry as shown.

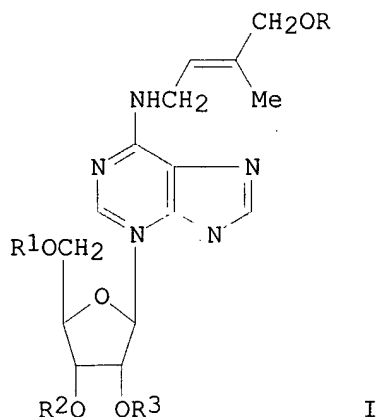


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 113:172616 The synthesis of phosphorus derivatives of ribosyl zeatin. Shadid, Belal; Van der Plas, Henk C. (Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.). Tetrahedron, 46(6), 2179-86 (English) 1990. CODEN: TETRAB. ISSN: 0040-4020.

GI



AB Sulfur was used for the conversion of ribosyl zeatin phosphonate I [R = PH(O)OH, R1 = SiMe2CMe3, PH(O)OH, R2R3 = CHOMe] (II) into the corresponding thiophosphates I [R = P(S)(OH)2]. 2,2'-Dipyridyldisulfide in the presence of MeOH was used for the conversion of II into the corresponding Me phosphates I [R = P(O)(OH)OMe]. Deprotection of these compds. gave the phosphorus derivs. of ribosyl zeatin I [R, R1 = H, PH(O)OH, P(O)(OH)OMe, P(S)(OH)2; R2 = R3 = H].

L5 ANSWER 62 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 129788-95-0 REGISTRY

CN 5'-Adenylic acid, N-[4-[(hydroxymethoxyphosphinyl)oxy]-3-methyl-2-butenyl]-, 5'-methyl ester, (E)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C17 H27 N5 O11 P2

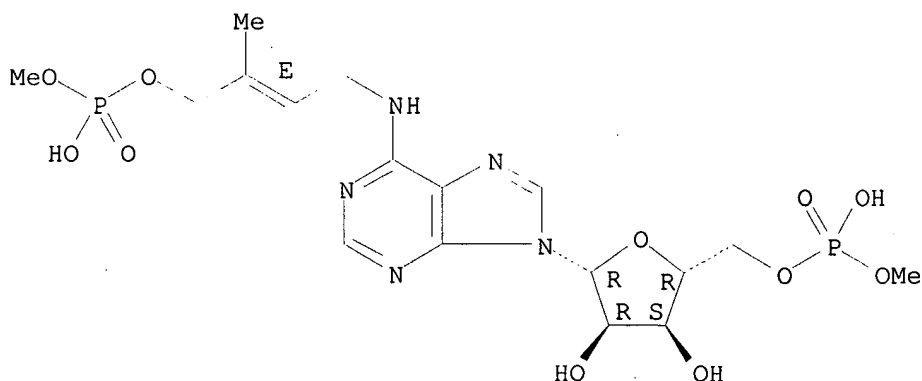
SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

Absolute stereochemistry.

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

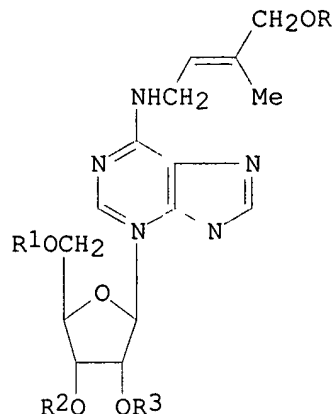
1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

Searched by: Mary Hale 308-4258 CM-1 1E01

REFERENCE 1: 113:172616 The synthesis of phosphorus derivatives of ribosyl zeatin. Shadid, Belal; Van der Plas, Henk C. (Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.). Tetrahedron, 46(6), 2179-86 (English) 1990. CODEN: TETRAB. ISSN: 0040-4020.

GI



I

AB Sulfur was used for the conversion of ribosyl zeatin phosphonate I [R = PH(O)OH, R1 = SiMe2CMe3, PH(O)OH, R2R3 = CHOMe] (II) into the corresponding thiophosphates I [R = P(S)(OH)2]. 2,2'-Dipyridyldisulfide in the presence of MeOH was used for the conversion of II into the corresponding Me phosphates I [R = P(O)(OH)OMe]. Deprotection of these compds. gave the phosphorus derivs. of ribosyl zeatin I [R, R1 = H, PH(O)OH, P(O)(OH)OMe, P(S)(OH)2; R2 = R3 = H].

L5 ANSWER 63 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 129788-94-9 REGISTRY

CN 5'-Adenylic acid, N-[4-[(hydroxymethoxyphosphinyl)oxy]-3-methyl-2-butenyl]-2',3'-O-(methoxymethylene)-, 5'-methyl ester, (E)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Furo[3,4-d]-1,3-dioxole, 5'-adenylic acid deriv.

FS STEREOSEARCH

MF C19 H29 N5 O12 P2

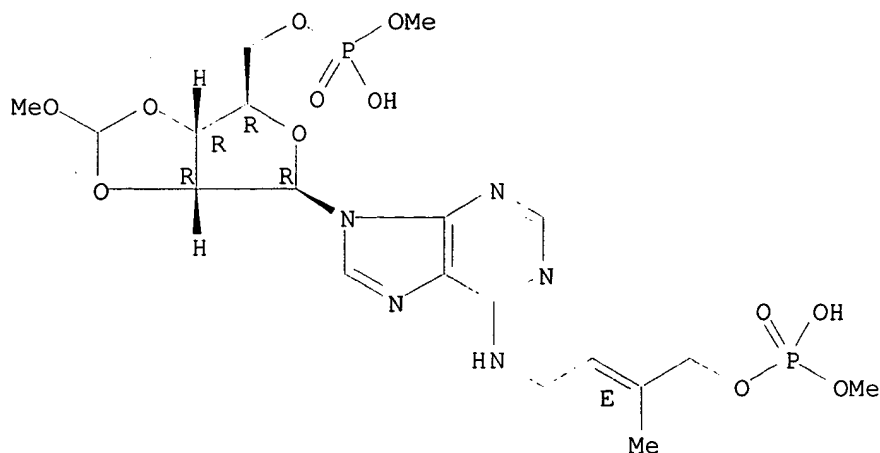
SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

Absolute stereochemistry.

Double bond geometry as shown.

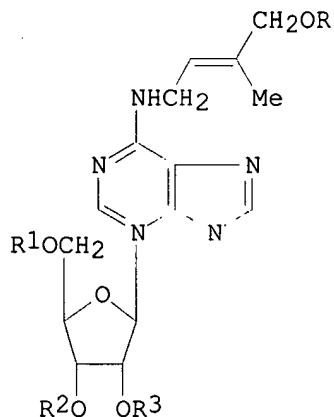


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 113:172616 The synthesis of phosphorus derivatives of ribosyl zeatin. Shadid, Belal; Van der Plas, Henk C. (Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.). Tetrahedron, 46(6), 2179-86 (English) 1990. CODEN: TETRAB. ISSN: 0040-4020.

GI



I

AB Sulfur was used for the conversion of ribosyl zeatin phosphonate I [R = PH(O)OH, R1 = SiMe2CMe3, PH(O)OH, R2R3 = CHOMe] (II) into the corresponding thiophosphates I [R = P(S)(OH)2]. 2,2'-Dipyridyldisulfide in the presence of MeOH was used for the conversion of II into the corresponding Me phosphates I [R = P(O)(OH)OMe]. Deprotection of these compds. gave the phosphorus derivs. of ribosyl zeatin I [R, R1 = H, PH(O)OH, P(O)(OH)OMe, P(S)(OH)2; R2 = R3 = H].

L5 ANSWER 64 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 129788-93-8 REGISTRY

CN Adenosine, N-[4-[(hydroxymercaptophosphinyl)oxy]-3-methyl-2-butenyl]-2',3'-O-(methoxymethylene)-, 5'-(dihydrogen phosphorothioate), (E)- (9CI) (CA

Searched by: Mary Hale 308-4258 CM-1 1E01

INDEX NAME)

OTHER CA INDEX NAMES:

CN Furo[3,4-d]-1,3-dioxole, adenosine deriv.

FS STEREOSEARCH

MF C17 H25 N5 O10 P2 S2

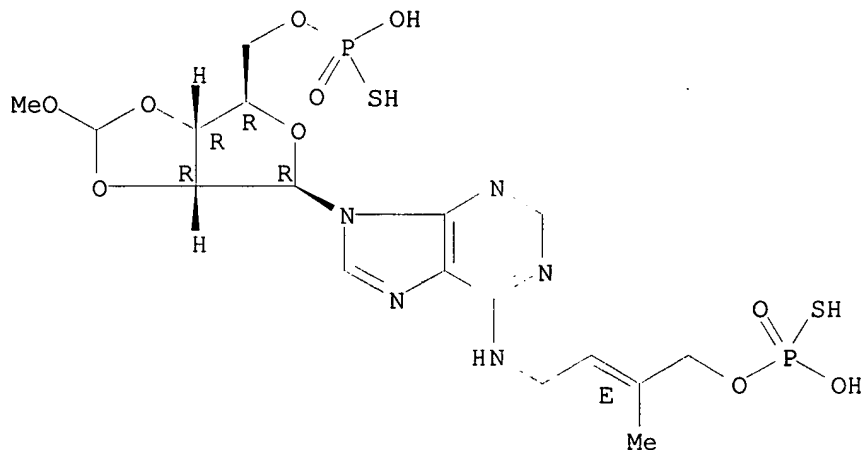
SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

Absolute stereochemistry.

Double bond geometry as shown.



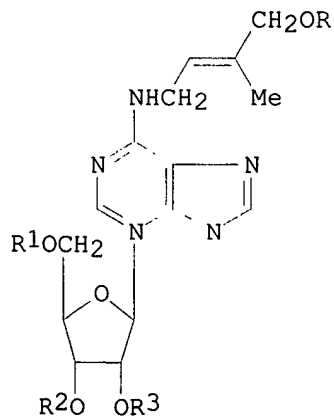
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 113:172616 The synthesis of phosphorus derivatives of ribosyl zeatin. Shadid, Belal; Van der Plas, Henk C. (Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.). Tetrahedron, 46(6), 2179-86 (English) 1990. CODEN: TETRAB. ISSN: 0040-4020.

GI



I

AB Sulfur was used for the conversion of ribosyl zeatin phosphonate I [R = PH(O)OH, R1 = SiMe2CMe3, PH(O)OH, R2R3 = CHOMe] (II) into the corresponding thiophosphates I [R=P(S)(OH)2]. 2,2'-Dipyridyldisulfide in the presence of MeOH was used for the conversion of II into the corresponding Me phosphates I [R = P(O)(OH)OMe]. Deprotection of these compds. gave the phosphorus derivs. of ribosyl zeatin I [R, R1 = H, PH(O)OH, P(O)(OH)OMe, P(S)(OH)2; R2 = R3 = H].

L5 ANSWER 65 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 129788-92-7 REGISTRY

CN Adenosine, 5'-O-[(1,1-dimethylethyl)dimethylsilyl]-N-[4-[(hydroxymethoxyphosphinyl)oxy]-3-methyl-2-butenyl]-2',3'-O-(methoxymethylene)-, (E)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Furo[3,4-d]-1,3-dioxole, adenosine deriv.

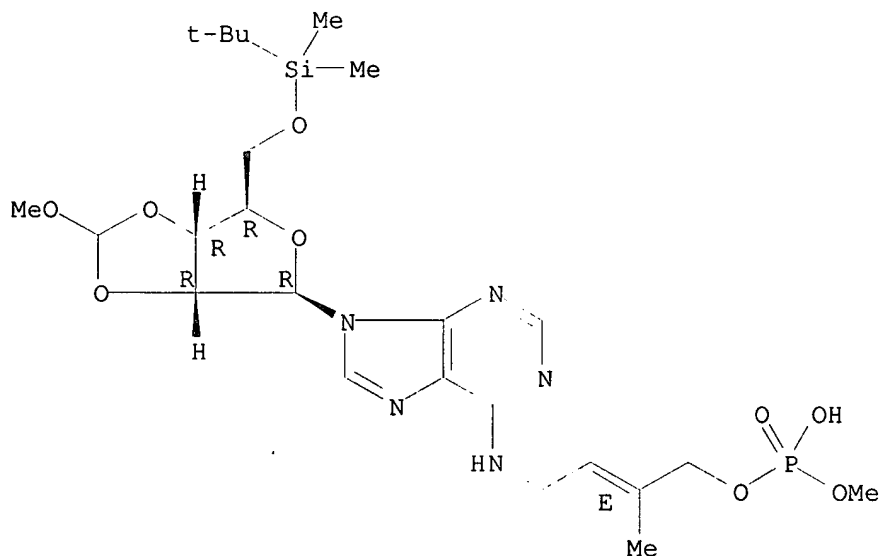
FS STEREOSEARCH

MF C24 H40 N5 O9 P Si

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

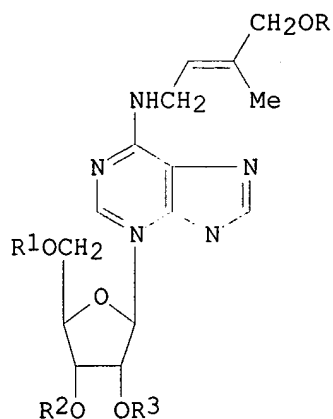
1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 113:172616 The synthesis of phosphorus derivatives of ribosyl zeatin. Shadid, Belal; Van der Plas, Henk C. (Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.). Tetrahedron, 46(6), 2179-86 (English) 1990. CODEN: TETRAB. ISSN: 0040-4020.

GI

Searched by: Mary Hale 308-4258 CM-1 1E01



I

AB Sulfur was used for the conversion of ribosyl zeatin phosphonate I [R = PH(O)OH, R1 = SiMe2CMe3, PH(O)OH, R2R3 = CHOMe] (II) into the corresponding thiophosphates I [R = P(S)(OH)2]. 2,2'-Dipyridyldisulfide in the presence of MeOH was used for the conversion of II into the corresponding Me phosphates I [R = P(O)(OH)OMe]. Deprotection of these compds. gave the phosphorus derivs. of ribosyl zeatin I [R, R1 = H, PH(O)OH, P(O)(OH)OMe, P(S)(OH)2; R2 = R3 = H].

L5 ANSWER 66 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 129788-91-6 REGISTRY

CN Adenosine, N-[4-[(hydroxymercaptophosphinyl)oxy]-3-methyl-2-butenyl]-5'-O-[(1,1-dimethylethyl)dimethylsilyl]-2',3'-O-(methoxymethylene)-, (E)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Furo[3,4-d]-1,3-dioxole, adenosine deriv.

FS STEREOSEARCH

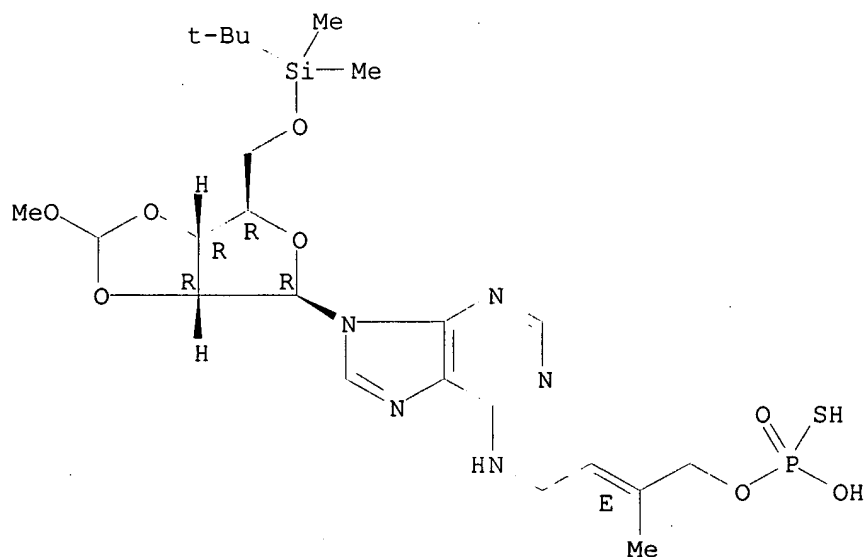
MF C23 H38 N5 O8 P S Si

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Double bond geometry as shown.

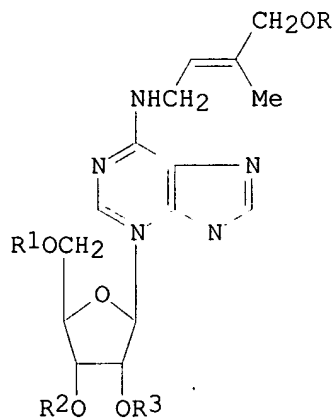


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 113:172616 The synthesis of phosphorus derivatives of ribosyl zeatin. Shadid, Belal; Van der Plas, Henk C. (Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.). Tetrahedron, 46(6), 2179-86 (English) 1990. CODEN: TETRAB. ISSN: 0040-4020.

GI



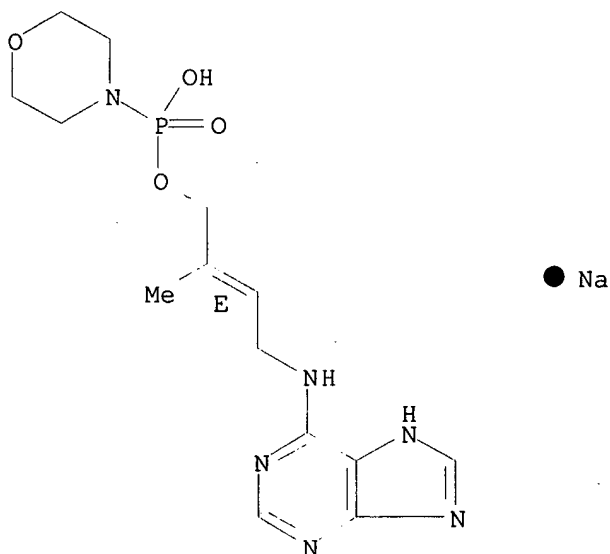
I

AB Sulfur was used for the conversion of ribosyl zeatin phosphonate I [R = PH(O)OH, R1 = SiMe2CMe3, PH(O)OH, R2R3 = CHOMe] (II) into the corresponding thiophosphates I [R = P(S)(OH)2]. 2,2'-Dipyridyldisulfide in the presence of MeOH was used for the conversion of II into the corresponding Me phosphates I [R = P(O)(OH)OMe]. Deprotection of these compds. gave the phosphorus derivs. of ribosyl zeatin I [R, R1 = H, PH(O)OH, P(O)(OH)OMe, P(S)(OH)2; R2 = R3 = H].

Searched by: Mary Hale 308-4258 CM-1 1E01

L5 ANSWER 67 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 128429-15-2 REGISTRY
 CN Phosphonic acid, 4-morpholinyl-, mono[2-methyl-4-(1H-purin-6-ylamino)-2-butenyl] ester, monosodium salt, (E)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C14 H21 N6 O4 P . Na
 SR CA
 LC STN Files: BEILSTEIN*, CA, CAPLUS
 (*File contains numerically searchable property data)
 CRN (128429-13-0)

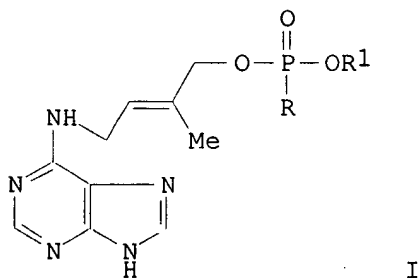
Double bond geometry as shown.



1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 113:58779 A convenient new synthesis of the allylic pyrophosphate of trans-zeatin. Shadid, Belal; Van der Plas, Henk C. (Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.). Tetrahedron, 46(3), 895-900 (English) 1990. CODEN: TETRAB. ISSN: 0040-4020.

GI



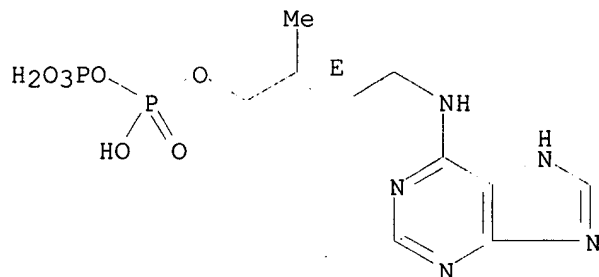
AB trans-Zeatin phosphonate I (R = R1 = H) was converted into the

Searched by: Mary Hale 308-4258 CM-1 1E01

phosphoromorpholidate, which on treatment with the $\text{Bu}_3\text{NOP}(\text{O})(\text{OH})_2$ gave the allylic pyrophosphate I [$\text{R} = \text{OH}$, $\text{R}_1 = \text{P}(\text{O})(\text{OH})_2$].

L5 ANSWER 68 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 128429-14-1 REGISTRY
CN Diphosphoric acid, mono[2-methyl-4-(1H-purin-6-ylamino)-2-butenyl] ester,
(E)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C10 H15 N5 O7 P2
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Double bond geometry as shown.

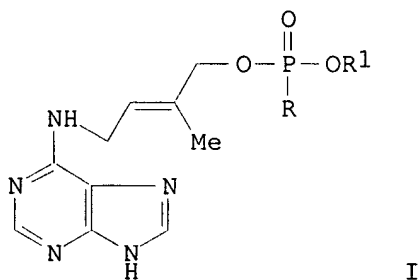


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 113:58779 A convenient new synthesis of the allylic pyrophosphate of trans-zeatin. Shadid, Belal; Van der Plas, Henk C. (Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.). Tetrahedron, 46(3), 895-900 (English) 1990. CODEN: TETRAB. ISSN: 0040-4020.

GI



I

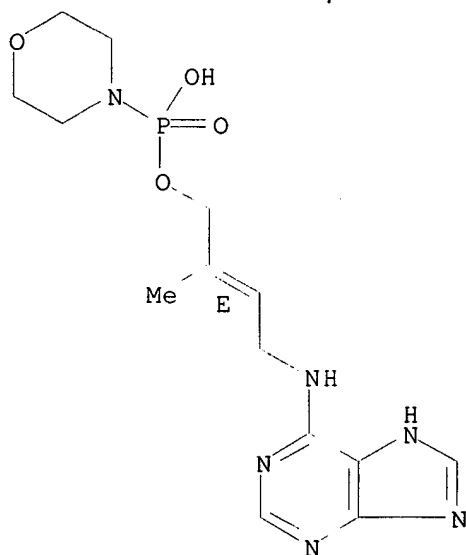
AB trans-Zeatin phosphonate I ($\text{R} = \text{R}_1 = \text{H}$) was converted into the phosphoromorpholidate, which on treatment with the $\text{Bu}_3\text{NOP}(\text{O})(\text{OH})_2$ gave the allylic pyrophosphate I [$\text{R} = \text{OH}$, $\text{R}_1 = \text{P}(\text{O})(\text{OH})_2$].

L5 ANSWER 69 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 128429-13-0 REGISTRY
CN Phosphonic acid, 4-morpholinyl-, mono[2-methyl-4-(1H-purin-6-ylamino)-2-butenyl] ester, (E)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH

Searched by: Mary Hale 308-4258 CM-1 1E01

MF C14 H21 N6 O4 P
 CI COM
 SR CA
 LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
 (*File contains numerically searchable property data)

Double bond geometry as shown.

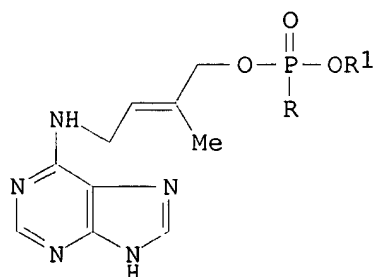


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 113:58779 A convenient new synthesis of the allylic pyrophosphate of trans-zeatin. Shadid, Belal; Van der Plas, Henk C. (Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.). Tetrahedron, 46(3), 895-900 (English) 1990. CODEN: TETRAB. ISSN: 0040-4020.

GI



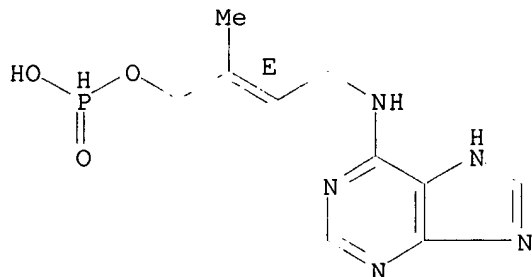
I

AB trans-Zeatin phosphonate I (R = R1 = H) was converted into the phosphoromorpholidate, which on treatment with the Bu3NOP(O)(OH)2 gave the allylic pyrophosphate I [R = OH, R1 = P(O)(OH)2].

Searched by: Mary Hale 308-4258 CM-1 1E01

L5 ANSWER 70 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 128429-12-9 REGISTRY
 CN Phosphonic acid, [2-methyl-4-(1H-purin-6-ylamino)-2-butenyl] ester, monosodium salt, (E)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C10 H14 N5 O3 P . Na
 SR CA
 LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
 (*File contains numerically searchable property data)
 CRN (124061-45-6)

Double bond geometry as shown.

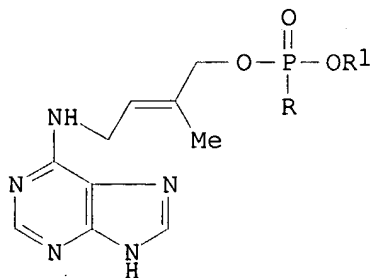


● Na

1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 113:58779 A convenient new synthesis of the allylic pyrophosphate of trans-zeatin. Shadid, Belal; Van der Plas, Henk C. (Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.). Tetrahedron, 46(3), 895-900 (English) 1990. CODEN: TETRAB. ISSN: 0040-4020.

GI



I

AB trans-Zeatin phosphonate I (R = R1 = H) was converted into the phosphoromorpholidate, which on treatment with the Bu3NOP(O)(OH)2 gave the allylic pyrophosphate I [R = OH, R1 = P(O)(OH)2].

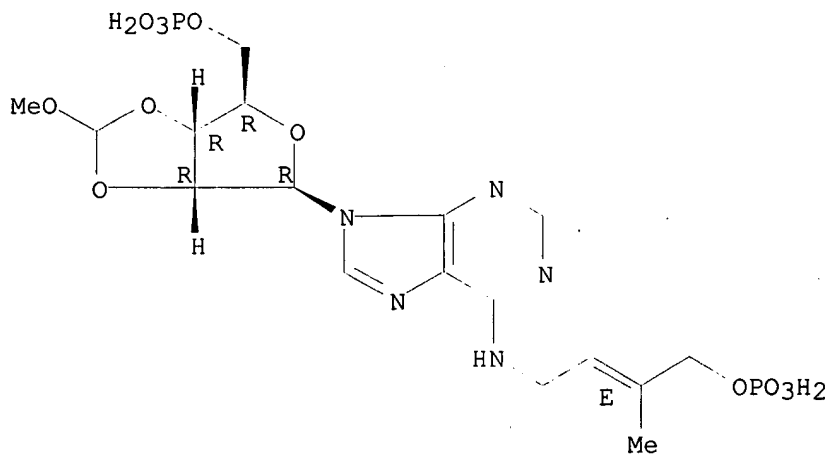
L5 ANSWER 71 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 128198-65-2 REGISTRY
 CN 5'-Adenylic acid, 2',3'-O-(methoxymethylene)-N-[3-methyl-4-(phosphonooxy)-2-butenyl]-, (E)- (9CI) (CA INDEX NAME)

Searched by: Mary Hale 308-4258 CM-1 1E01

OTHER CA INDEX NAMES:

CN Furo[3,4-d]-1,3-dioxole, 5'-adenylic acid deriv.
FS STEREOSEARCH
MF C17 H25 N5 O12 P2
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.

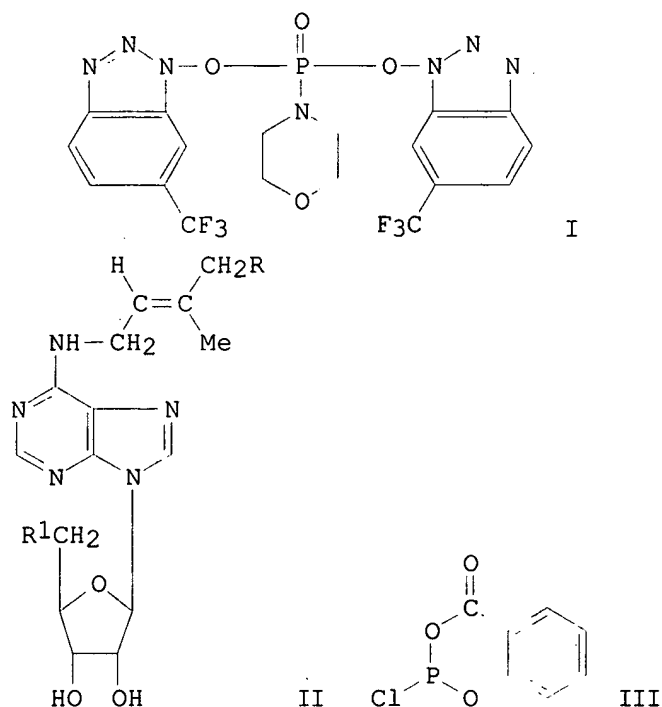


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 113:59752 The synthesis of cytokinin phosphates. Shadid, Belal; Van der Plas, Henk C. (Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.). Tetrahedron, 46(3), 901-12 (English) 1990. CODEN: TETRAB. ISSN: 0040-4020.

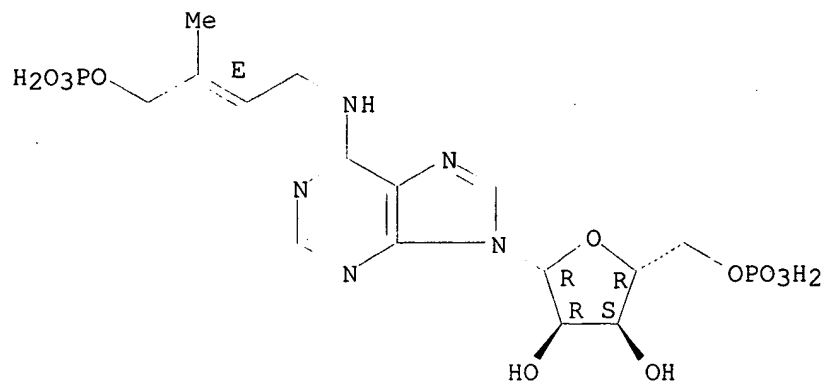
GI



AB The bifunctional phosphorylating reagent N-morpholino O,O-bis[6-(trifluoromethyl)benzotriazolyl]phosphate I was used for the prepn. of adenosine phosphates II (R = OH, OPO₃H₂, R₁ = OPO₃H₂), whereas the monofunctional phosphitylating reagent 2-chlorobenzodioxaphosphorin-3-one III was used for the prepn. of ribosyl zeatin allylic phosphate II (R = OPO₃H₂, R₁ = H) and ribosyl zeatin diphosphate II (R = R₁ = OPO₃H₂).

L5 ANSWER 72 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 128185-01-3 REGISTRY
 CN 5'-Adenylic acid, N-[3-methyl-4-(phosphonooxy)-2-butenyl]-, (E)- (9CI)
 (CA INDEX NAME)
 FS STEREOSEARCH
 MF C15 H23 N5 O11 P2
 CI COM
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.
 Double bond geometry as shown.



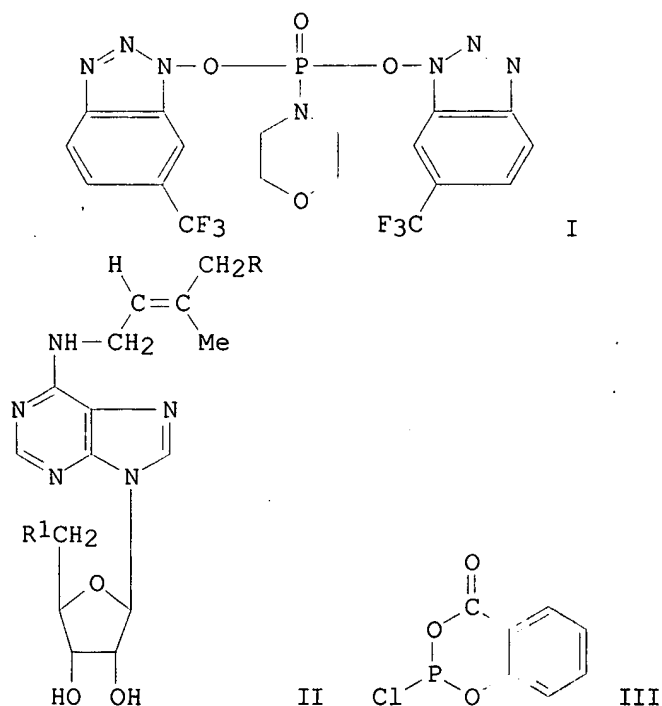
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 113:59752 The synthesis of cytokinin phosphates. Shadid, Belal; Van der Plas, Henk C. (Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.). Tetrahedron, 46(3), 901-12 (English) 1990. CODEN: TETRAB. ISSN: 0040-4020.

GI



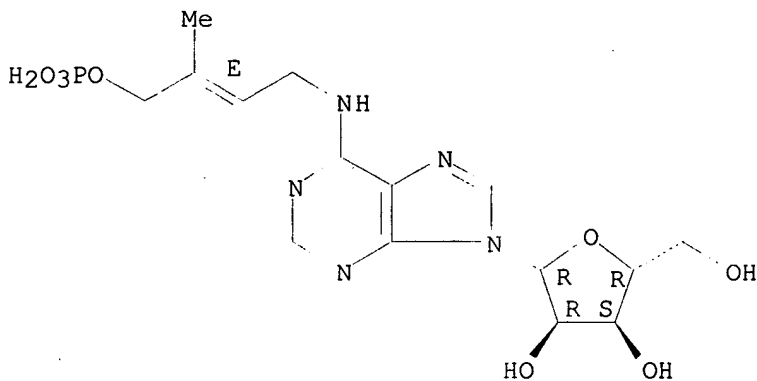
AB The bifunctional phosphorylating reagent N-morpholino O,O-bis[6-trifluoromethyl)benzotriazolyl]phosphate I was used for the prepn. of

Searched by: Mary Hale 308-4258 CM-1 1E01

adenosine phosphates II (R = OH, OPO₃H₂, R₁ = OPO₃H₂), whereas the monofunctional phosphitylating reagent 2-chlorobenzodioxaphosphorin-3-one III was used for the prepn. of ribosyl zeatin allylic phosphate II (R = OPO₃H₂, R₁ = H) and ribosyl zeatin diphosphate II (R = R₁ = OPO₃H₂).

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L5 ANSWER 73 OF 140  REGISTRY  COPYRIGHT 2002 ACS
RN 128185-00-2  REGISTRY
CN Adenosine, N-[3-methyl-4-(phosphonooxy)-2-butenyl]-, (E)- (9CI)  (CA INDEX
NAME)
FS STEREOSEARCH
MF C15 H22 N5 O8 P
CI COM
SR CA
LC STN Files:  CA, CAPLUS, CASREACT
```

Absolute stereochemistry.
Double bond geometry as shown.

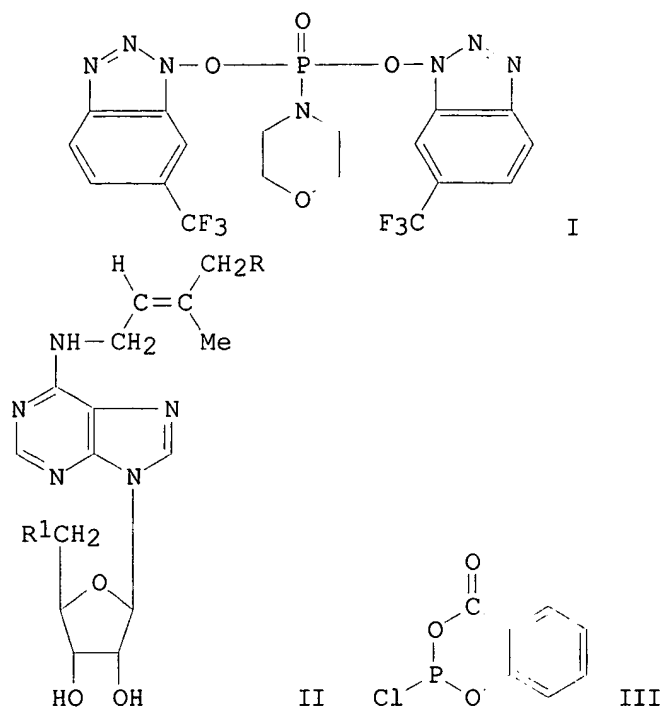


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 113:59752 The synthesis of cytokinin phosphates. Shadid, Belal; Van der Plas, Henk C. (Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.). Tetrahedron, 46(3), 901-12 (English) 1990. CODEN: TETRAB. ISSN: 0040-4020.

GI



AB The bifunctional phosphorylating reagent N-morpholino O,O-bis[6-(trifluoromethyl)benzotriazolyl]phosphate I was used for the prepn. of adenosine phosphates II (R = OH, OPO₃H₂, R₁ = OPO₃H₂), whereas the monofunctional phosphitylating reagent 2-chlorobenzodioxaphosphorin-3-one III was used for the prepn. of ribosyl zeatin allylic phosphate II (R = OPO₃H₂, R₁ = H) and ribosyl zeatin diphosphate II (R = R₁ = OPO₃H₂).

L5 ANSWER 74 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 128184-99-6 REGISTRY

CN Adenosine, 5'-O-[(1,1-dimethylethyl)dimethylsilyl]-2',3'-O-(methoxymethylene)-N-[3-methyl-4-(phosphonooxy)-2-butenyl]-, (E)- (9CI)
(CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Furo[3,4-d]-1,3-dioxole, adenosine deriv.

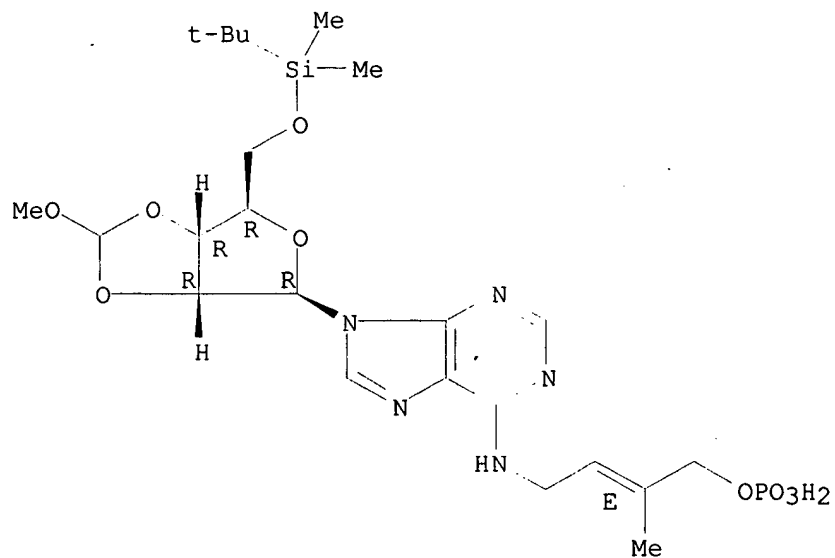
FS STEREOSEARCH

MF C23 H38 N5 O9 P Si

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.

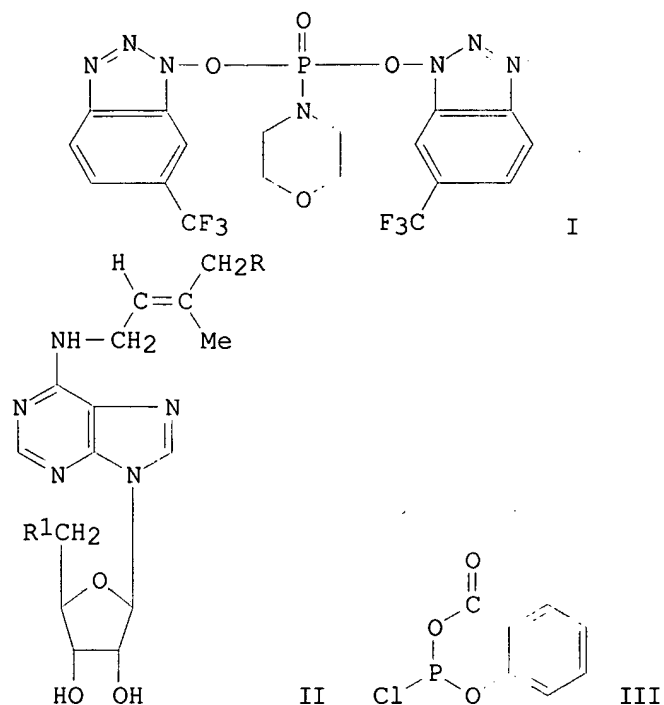


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 113:59752 The synthesis of cytokinin phosphates. Shadid, Belal; Van der Plas, Henk C. (Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.). Tetrahedron, 46(3), 901-12 (English) 1990. CODEN: TETRAB. ISSN: 0040-4020.

GI



AB The bifunctional phosphorylating reagent N-morpholino O,O-bis[6-(trifluoromethyl)benzotriazolyl]phosphate I was used for the prepn. of adenosine phosphates II (R = OH, OPO₃H₂, R₁ = OPO₃H₂), whereas the monofunctional phosphitylating reagent 2-chlorobenzodioxaphosphorin-3-one III was used for the prepn. of ribosyl zeatin allylic phosphate II (R = OPO₃H₂, R₁ = H) and ribosyl zeatin diphosphate II (R = R₁ = OPO₃H₂).

L5 ANSWER 75 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 128184-98-5 REGISTRY

CN Adenosine, N-[4-[(hydroxyphosphinyl)oxy]-3-methyl-2-butenyl]-2',3'-O-(methoxymethylene)-, 5'-(hydrogen phosphonate), (E)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Furo[3,4-d]-1,3-dioxole, adenosine deriv.

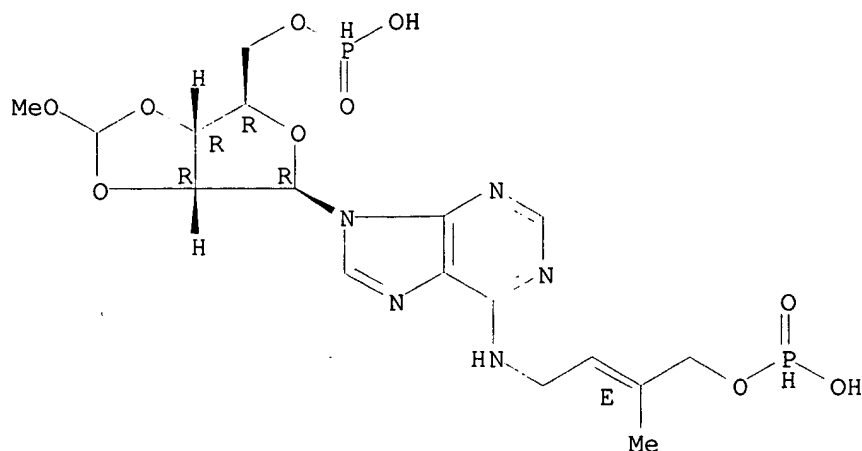
FS STEREOSEARCH

MF C17 H25 N5 O10 P2

SR CA

LC STN Files: CA, CAPLUS

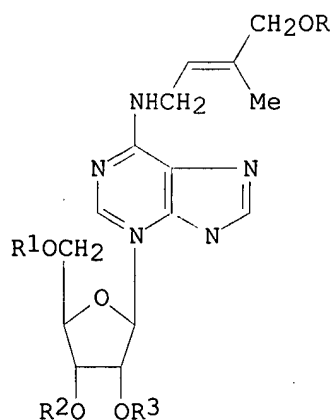
Absolute stereochemistry.
Double bond geometry as shown.



2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 113:172616 The synthesis of phosphorus derivatives of ribosyl zeatin. Shadid, Belal; Van der Plas, Henk C. (Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.). Tetrahedron, 46(6), 2179-86 (English) 1990. CODEN: TETRAB. ISSN: 0040-4020.

GI



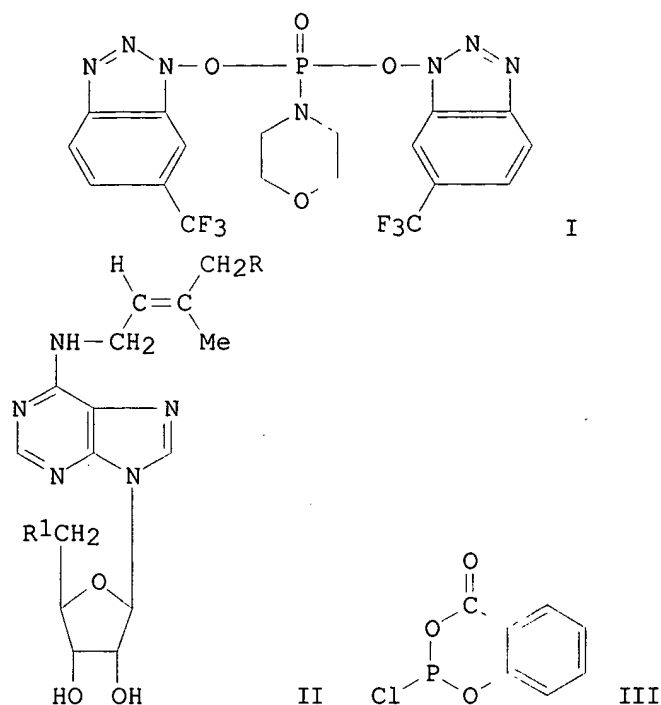
I

AB Sulfur was used for the conversion of ribosyl zeatin phosphonate I [R = PH(O)OH, R1 = SiMe2CMe3, PH(O)OH, R2R3 = CHOMe] (II) into the corresponding thiophosphates I [R = P(S)(OH)2]. 2,2'-Dipyridyldisulfide in the presence of MeOH was used for the conversion of II into the corresponding Me phosphates I [R = P(O)(OH)OMe]. Deprotection of these compds. gave the phosphorus derivs. of ribosyl zeatin I [R, R1 = H, PH(O)OH, P(O)(OH)OMe, P(S)(OH)2; R2 = R3 = H].

REFERENCE 2: 113:59752 The synthesis of cytokinin phosphates. Shadid, Belal; Van der Plas, Henk C. (Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.). Tetrahedron, 46(3), 901-12 (English) 1990. CODEN: TETRAB. ISSN: 0040-4020.

GI

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AB The bifunctional phosphorylating reagent N-morpholino 0,0-bis[6-(trifluoromethyl)benzotriazolyl]phosphate I was used for the prepn. of adenosine phosphates II (R = OH, OPO₃H₂, R₁ = OPO₃H₂), whereas the monofunctional phosphitylating reagent 2-chlorobenzodioxaphosphorin-3-one III was used for the prepn. of ribosyl zeatin allylic phosphate II (R = OPO₃H₂, R₁ = H) and ribosyl zeatin diphosphate II (R = R₁ = OPO₃H₂).

L5 ANSWER 76 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 128184-97-4 REGISTRY

CN Adenosine, 5'-O-[(1,1-dimethylethyl)dimethylsilyl]-N-[4-[(hydroxyphosphinyl)oxy]-3-methyl-2-butenyl]-2',3'-O-(methoxymethylene)-, (E)- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Furo[3,4-d]-1,3-dioxole, adenosine deriv.

FS STEREOSEARCH

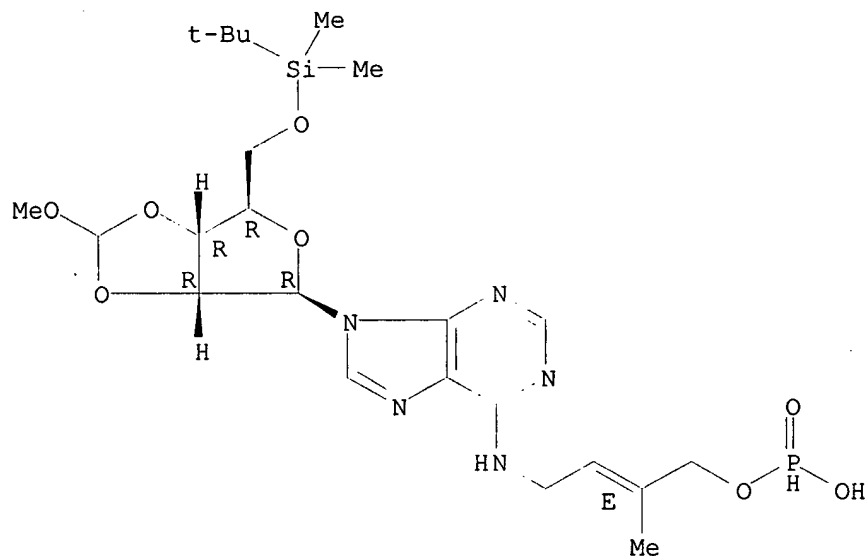
MF C23 H38 N5 O8 P Si

SR CA

LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.

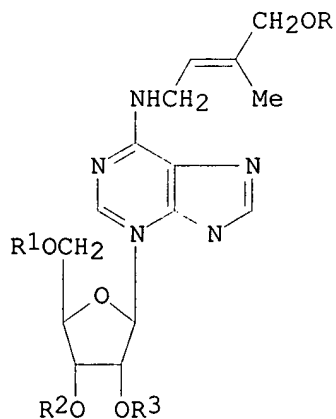
Double bond geometry as shown.



2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 113:172616 The synthesis of phosphorus derivatives of ribosyl zeatin. Shadid, Belal; Van der Plas, Henk C. (Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.). Tetrahedron, 46(6), 2179-86 (English) 1990. CODEN: TETRAB. ISSN: 0040-4020.

GI



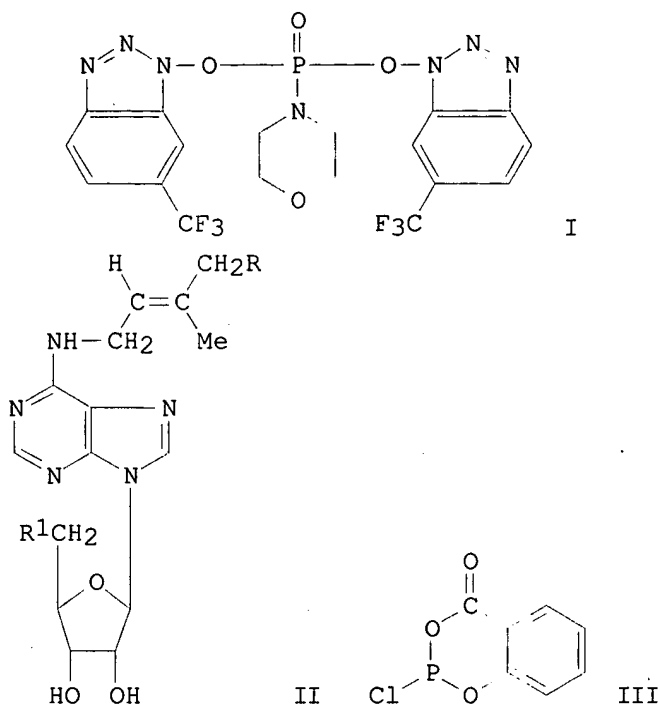
I

AB Sulfur was used for the conversion of ribosyl zeatin phosphonate I [R = PH(O)OH, R1 = SiMe2CMe3, PH(O)OH, R2R3 = CHOMe] (II) into the corresponding thiophosphates I [R = P(S)(OH)2]. 2,2'-Dipyridyldisulfide in the presence of MeOH was used for the conversion of II into the corresponding Me phosphates I [R = P(O)(OH)OMe]. Deprotection of these compds. gave the phosphorus derivs. of ribosyl zeatin I [R, R1 = H, PH(O)OH, P(O)(OH)OMe, P(S)(OH)2; R2 = R3 = H].

REFERENCE 2: 113:59752 The synthesis of cytokinin phosphates. Shadid, Belal; Van der Plas, Henk C. (Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.). Tetrahedron, 46(3), 901-12 (English) 1990.

Searched by: Mary Hale 308-4258 CM-1 1E01

GI



AB The bifunctional phosphorylating reagent N-morpholino O,O-bis[6-trifluoromethyl)benzotriazolyl]phosphate I was used for the prepn. of adenosine phosphates II (R = OH, OPO₃H₂, R₁ = OPO₃H₂), whereas the monofunctional phosphitylating reagent 2-chlorobenzodioxaphosphorin-3-one III was used for the prepn. of ribosyl zeatin allylic phosphate II (R = OPO₃H₂, R₁ = H) and ribosyl zeatin diphosphate II (R = R₁ = OPO₃H₂).

L5 ANSWER 77 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 128059-50-7 REGISTRY

CN 5'-Adenylic acid, N-[3-methyl-4-(phosphonooxy)-2-butenyl]-, sodium salt, (E)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C15 H23 N5 O11 P2 . x Na

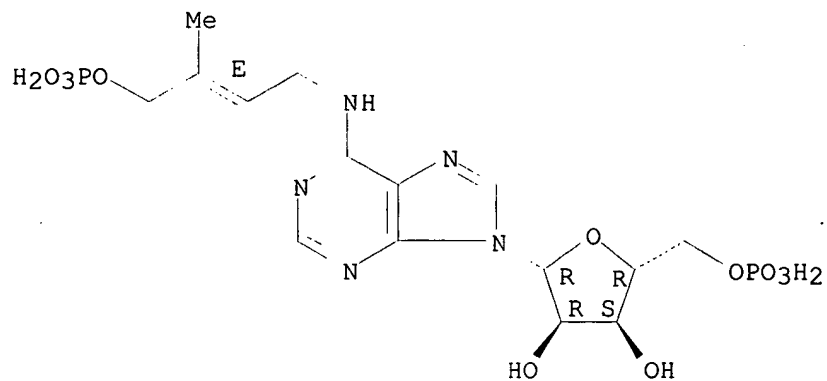
SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

CRN (128185-01-3)

Absolute stereochemistry.
Double bond geometry as shown.

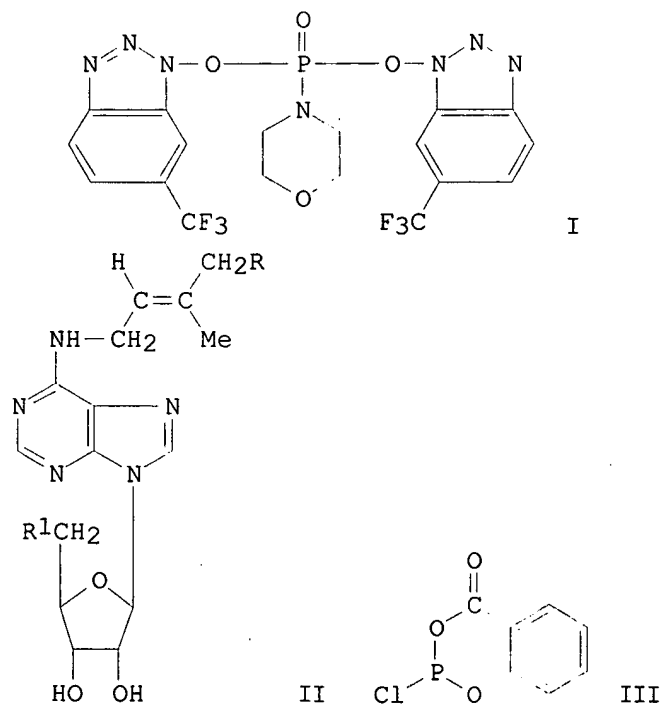


●x Na

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 113:59752 The synthesis of cytokinin phosphates. Shadid, Belal; Van der Plas, Henk C. (Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.). Tetrahedron, 46(3), 901-12 (English) 1990. CODEN: TETRAB. ISSN: 0040-4020.

GI



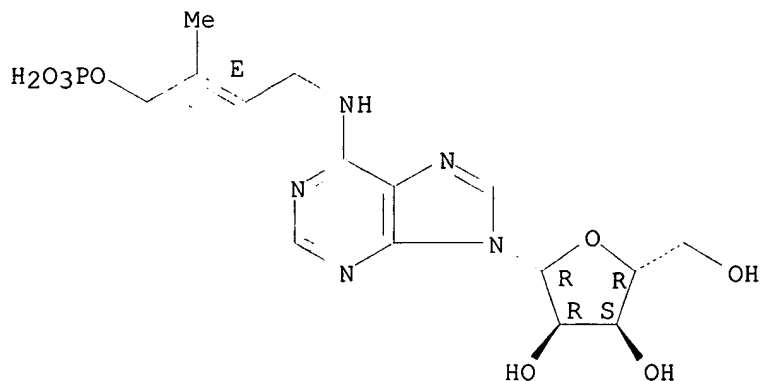
AB The bifunctional phosphorylating reagent N-morpholino O,O-bis[6-

Searched by: Mary Hale 308-4258 CM-1 1E01

trifluoromethyl)benzotriazolyl]phosphate I was used for the prepn. of adenosine phosphates II (R = OH, OPO₃H₂, R₁ = OPO₃H₂), whereas the monofunctional phosphitylating reagent 2-chlorobenzodioxaphosphorin-3-one III was used for the prepn. of ribosyl zeatin allylic phosphate II (R = OPO₃H₂, R₁ = H) and ribosyl zeatin diphosphate II (R = R₁ = OPO₃H₂).

L5 ANSWER 78 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 128059-49-4 REGISTRY
CN Adenosine, N-[3-methyl-4-(phosphonoxy)-2-butenyl]-, sodium salt, (E)-
(9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C15 H22 N5 O8 P . x Na
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)
CRN (128185-00-2)

Absolute stereochemistry.
Double bond geometry as shown.

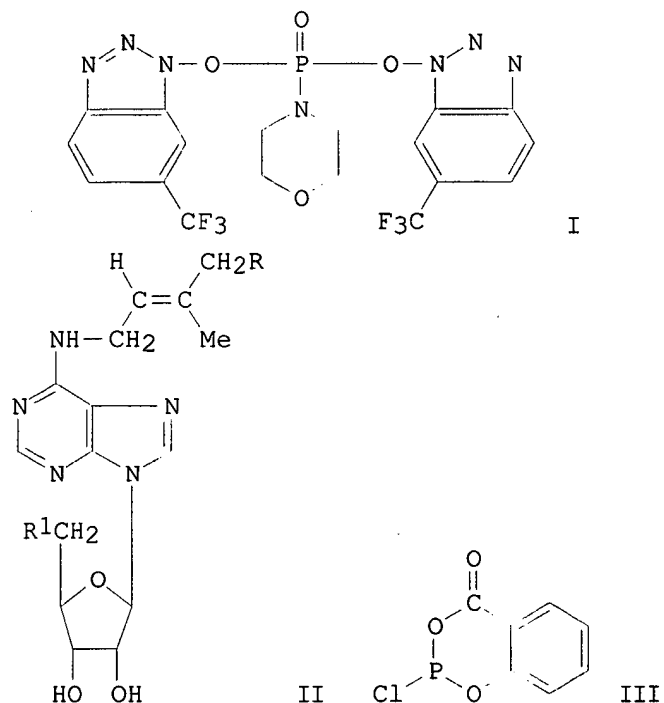


● x Na

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 113:59752 The synthesis of cytokinin phosphates. Shadid, Belal; Van der Plas, Henk C. (Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.). Tetrahedron, 46(3), 901-12 (English) 1990. CODEN: TETRAB. ISSN: 0040-4020.

GI



AB The bifunctional phosphorylating reagent N-morpholino O,O-bis[6-(trifluoromethyl)benzotriazolyl]phosphate I was used for the prepn. of adenosine phosphates II (R = OH, OPO₃H₂, R₁ = OPO₃H₂), whereas the monofunctional phosphitylating reagent 2-chlorobenzodioxaphosphorin-3-one III was used for the prepn. of ribosyl zeatin allylic phosphate II (R = OPO₃H₂, R₁ = H) and ribosyl zeatin diphosphate II (R = R₁ = OPO₃H₂).

L5 ANSWER 79 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 124061-45-6 REGISTRY

CN Phosphonic acid, mono[2-methyl-4-(1H-purin-6-ylamino)-2-butenyl] ester, (E)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C10 H14 N5 O3 P

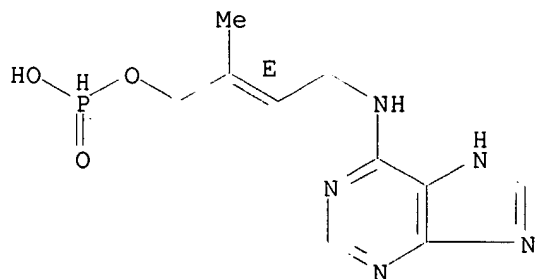
CI COM

SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT

(*File contains numerically searchable property data)

Double bond geometry as shown.



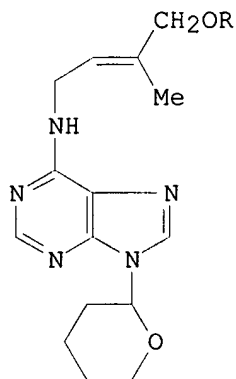
1 REFERENCES IN FILE CA (1967 TO DATE)

Searched by: Mary Hale 308-4258 CM-1 1E01

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 112:7250 The synthesis of allylic phosphate derivatives of trans zeatin. Shadid, Belal; Van der Plas, Henk C.; Vonk, C. R.; Davelaar, E.; Ribot, S. A. (Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.). Tetrahedron, 45(12), 3889-96 (English) 1989. CODEN: TETRAB. ISSN: 0040-4020.

GI



I

AB Phosphitylation of the allylic hydroxy group in 9-tetrahydropyranyl trans-zeatin (I, R = H) with salicyl chlorophosphate gives the allyl phosphonate I [R = P(O)(OH)H], which can be readily converted into I [R = P(S)(OH)2, P(O)(OMe)(OH), P(O)(OH)2]. After cleavage of the tetrahydropyranyl group under mild acidic conditions, allylic phosphate derivs. of trans-zeatin are obtained.

L5 ANSWER 80 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 124031-45-4 REGISTRY

CN 2-Buten-1-ol, 2-methyl-4-(1H-purin-6-ylamino)-, dihydrogen phosphorothioate (ester), (E)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

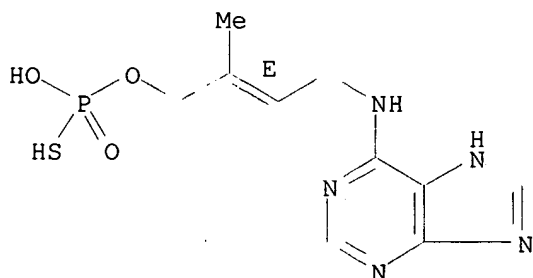
MF C10 H14 N5 O3 P S

SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT

(*File contains numerically searchable property data)

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

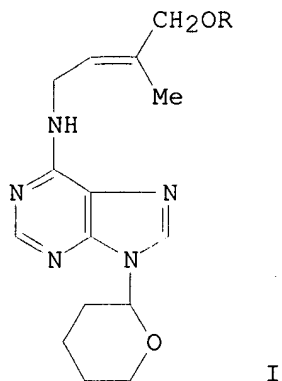
1 REFERENCES IN FILE CA (1967 TO DATE)

Searched by: Mary Hale 308-4258 CM-1 1E01

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 112:7250 The synthesis of allylic phosphate derivatives of trans zeatin. Shadid, Belal; Van der Plas, Henk C.; Vonk, C. R.; Davelaar, E.; Ribot, S. A. (Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.). Tetrahedron, 45(12), 3889-96 (English) 1989. CODEN: TETRAB. ISSN: 0040-4020.

GI



AB Phosphitylation of the allylic hydroxy group in 9-tetrahydropyranyl trans-zeatin (I, R = H) with salicyl chlorophosphite gives the allyl phosphonate I [R = P(O)(OH)H], which can be readily converted into I [R = P(S)(OH)2, P(O)(OMe)(OH), P(O)(OH)2]. After cleavage of the tetrahydropyranyl group under mild acidic conditions, allylic phosphate derivs. of trans-zeatin are obtained.

L5 ANSWER 81 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 124031-44-3 REGISTRY

CN 2-Buten-1-ol, 2-methyl-4-[[9-(tetrahydro-2H-pyran-2-yl)-9H-purin-6-yl]amino]-, dihydrogen phosphorothioate (ester), disodium salt, (E)- (9CI)
(CA INDEX NAME)

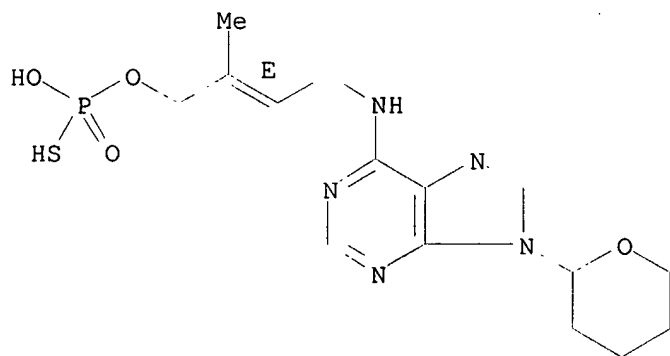
FS STEREOSEARCH

MF C15 H22 N5 O4 P S . 2 Na

SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)

. Double bond geometry as shown.

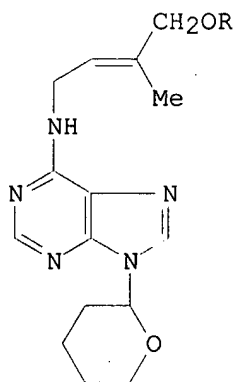


● 2 Na

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 112:7250 The synthesis of allylic phosphate derivatives of trans zeatin. Shadid, Belal; Van der Plas, Henk C.; Vonk, C. R.; Davelaar, E.; Ribot, S. A. (Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.). Tetrahedron, 45(12), 3889-96 (English) 1989. CODEN: TETRAB. ISSN: 0040-4020.

GI



I

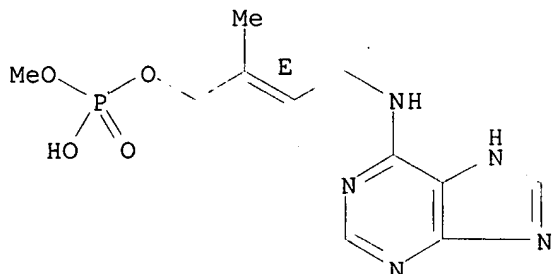
AB Phosphitylation of the allylic hydroxy group in 9-tetrahydropyranyll trans-zeatin (I, R = H) with salicyl chlorophosphate gives the allyl phosphonate I [R = P(O)(OH)H], which can be readily converted into I [R = P(S)(OH)2, P(O)(OMe)(OH), P(O)(OH)2]. After cleavage of the tetrahydropyranyll group under mild acidic conditions, allylic phosphate derivs. of trans-zeatin are obtained.

L5 ANSWER 82 OF 140 .REGISTRY COPYRIGHT 2002 ACS
RN 124031-43-2 REGISTRY
CN Phosphoric acid, monomethyl mono[2-methyl-4-(1H-purin-6-ylamino)-2-butenyl] ester, (E)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C11 H16 N5 O4 P
SR CA

Searched by: Mary Hale 308-4258 CM-1 1E01

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)

Double bond geometry as shown.



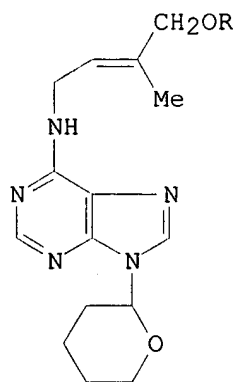
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 112:7250 The synthesis of allylic phosphate derivatives of trans zeatin. Shadid, Belal; Van der Plas, Henk C.; Vonk, C. R.; Davelaar, E.; Ribot, S. A. (Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.). Tetrahedron, 45(12), 3889-96 (English) 1989. CODEN: TETRAB. ISSN: 0040-4020.

GI



I

AB Phosphitylation of the allylic hydroxy group in 9-tetrahydropyranyl trans-zeatin (I, R = H) with salicyl chlorophosphite gives the allyl phosphonate I [R = P(O)(OH)H], which can be readily converted into I [R = P(S)(OH)₂, P(O)(OMe)(OH), P(O)(OH)₂]. After cleavage of the tetrahydropyranyl group under mild acidic conditions, allylic phosphate derivs. of trans-zeatin are obtained.

L5 ANSWER 83 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 124031-42-1 REGISTRY

CN Phosphoric acid, monomethyl mono[2-methyl-4-[[9-(tetrahydro-2H-pyran-2-yl)-9H-purin-6-yl]amino]-2-butenyl] ester, monosodium salt, (E)- (9CI) (CA INDEX NAME)

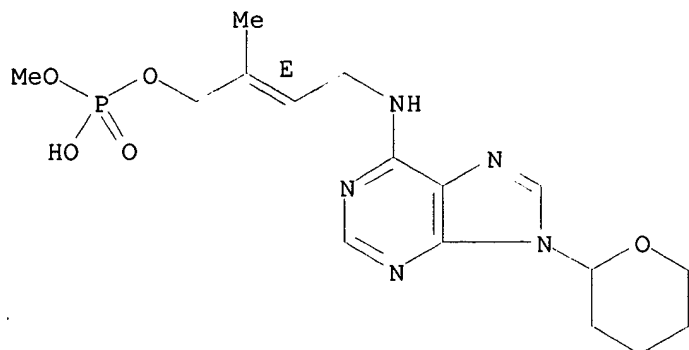
FS STEREOSEARCH

MF C16 H24 N5 O5 P . Na

Searched by: Mary Hale 308-4258 CM-1 1E01

SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)

Double bond geometry as shown.

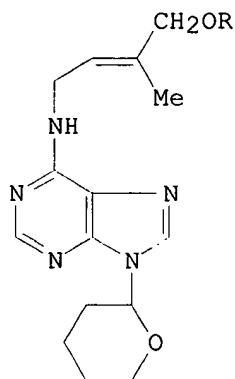


● Na

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 112:7250 The synthesis of allylic phosphate derivatives of trans zeatin. Shadid, Belal; Van der Plas, Henk C.; Vonk, C. R.; Davelaar, E.; Ribot, S. A. (Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.). Tetrahedron, 45(12), 3889-96 (English) 1989. CODEN: TETRAB. ISSN: 0040-4020.

GI



I

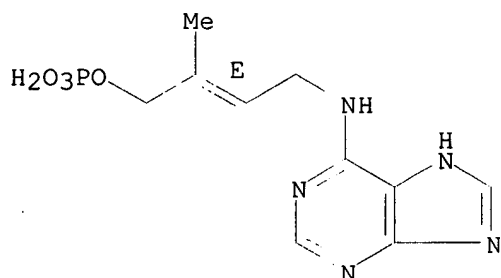
AB Phosphitylation of the allylic hydroxy group in 9-tetrahydropyranyl trans-zeatin (I, R = H) with salicyl chlorophosphate gives the allyl phosphonate I [R = P(O)(OH)H], which can be readily converted into I [R = P(S)(OH)₂, P(O)(OMe)(OH), P(O)(OH)₂]. After cleavage of the tetrahydropyranyl group under mild acidic conditions, allylic phosphate derivs. of trans-zeatin are obtained.

L5 ANSWER 84 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 124031-41-0 REGISTRY

Searched by: Mary Hale 308-4258 CM-1 1E01

CN 2-Buten-1-ol, 2-methyl-4-(1H-purin-6-ylamino)-, dihydrogen phosphate
(ester), (2E)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Buten-1-ol, 2-methyl-4-(1H-purin-6-ylamino)-, dihydrogen phosphate
(ester), (E)-
FS STEREOSEARCH
MF C10 H14 N5 O4 P
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1967 TO DATE)
4 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 135:354127 Cytokinin activity of zeatin allylic phosphate, a natural compound. Selivankina, S. Yu.; Karavaiko, N. N.; Kuiper, D.; Novikova, G. V.; Kulaeva, O. N. (Timiryazev Institute of Plant Physiology, Russian Academy of Sciences, Moscow, 127276, Russia). Plant Growth Regulation, 33(3), 157-164 (English) 2001. CODEN: PGRED3. ISSN: 0167-6903. Publisher: Kluwer Academic Publishers.

AB Zeatin allylic phosphate (ZAP) retarded chlorophyll loss in the barley leaf senescence assay at a concn. 20 times higher than for 6-benzyladenine (BA): the effective concns. for ZAP and BA were 10 μ M and 0.5 μ M, resp. Sodium molybdate, an inhibitor of phosphatases, decreased the ZAP effective concn. to 0.5 μ M without affecting leaf senescence and trans-zeatin activity in the control. This demonstrates the importance of the phosphate group for ZAP activity or its penetration into leaf cells. ZAP up-regulated the protein kinase activity of the barley leaf chromatin with concn. dependence similar to that of trans-zeatin. Conversely, ZAP was 1000 times less active than trans-zeatin in the competition with anti-idiotypic antibodies (raised against antibody to zeatin) for binding with a trans-zeatin-binding site of trans-zeatin-binding protein ZBP67 isolated from barley leaves. In contrast to trans-zeatin, ZAP did not activate RNA synthesis in the presence of ZBP in the in vitro system contg. chromatin and RNA polymerase I isolated from barley leaves. Thus, ZAP had cytokinin activity as demonstrated by the retardation of barley leaf senescence, but mol. target(s) for ZAP in barley leaf cells differs, at least partially, from these for trans-zeatin. Apparently, the cytokinin activity of ZAP results from its hydrolysis while producing zeatin.

REFERENCE 2: 119:4989 Zeatin allylic phosphate: occurrence, formation and possible role. Vonk, C. R.; Davelaar, E. (Cent. Agrobiol. Res., Wageningen, 6700 AA, Neth.). Curr. Plant Sci. Biotechnol. Agric., 13(Prog. Plant Growth Regul.), 617-23 (English) 1992. CODEN: CPBAE2. ISSN: 0924-1949.

Searched by: Mary Hale 308-4258 CM-1 1E01

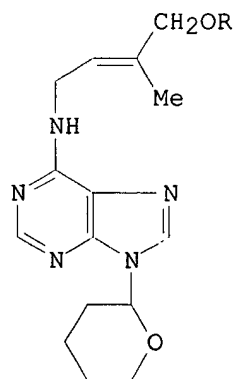
AB Formation of zeatin allylic phosphate (ZAP) by a biol. system has been demonstrated by incubation of a microsomal fraction prep'd. from bulb disks of iris and also by a microsomal fraction prep'd. in the same way from *Helianthus tuberosus*. Treatment of the microsomal fraction with Triton X-100 resulted in a sol. fraction showing ZAP-forming activity. This fraction was partially purified by Ultrogel HA-column chromatog. Ultrafree-MC filter units were used to further purify the ZAP-forming fraction, resulting in a five-fold increase in specific activity. Enzyme activity was optimal at a concn. of 4 μ g/mL of added partially purified microsomal protein and decreased at higher protein concn. The enzyme activity of Triton X-100 solubilized microsomal membranes was inhibited by pronase digestion (68% inhibition), and was completely destroyed in the presence of 0.5% SDS (final vol.) or after heat treatment (10 min, 100.degree.). The greatest quantity of ZAP-forming enzyme activity was present in the intracellular membrane fraction. This enzyme specifically recognizes the trans-form of zeatin rather than cis-zeatin or dihydrozeatin.

REFERENCE 3: 112:52323 Formation of zeatin allylic phosphate by the microsomal fractions of bulb disks of *Iris .times. hollandica* Tub. and tubers of *Helianthus tuberosus* L. Vonk, C. R.; Davelaar, E.; Ribot, S. A.; Shadid, B.; Van der Plas, H. C. (Cent. Agrobiol. Res., Wageningen, 6700 AA, Neth.). *Plant Growth Regul.*, 8(3), 263-76 (English) 1989. CODEN: PGRED3. ISSN: 0167-6903.

AB In bulbous *Iris*, zeatin originates from a nucleotide, zeatin-allylic-phosphate, in which a phosphate group is attached to the isoprenoid side-chain of zeatin. The formation of zeatin-allylic-phosphate from trans-zeatin and 8-[14C]-zeatin by the microsomal fractions of *Iris* bulb disks and *Helianthus tuberosus* were demonstrated. The responsible enzyme was partially purified. 5'-AMP was found to be a phosphate group-delivering substrate. Adenosine and adenine inhibited the enzyme reaction. The significance of the results is discussed in relation to cytokinin biosynthesis and the occurrence of bud blast in *Iris*.

REFERENCE 4: 112:7250 The synthesis of allylic phosphate derivatives of trans zeatin. Shadid, Belal; Van der Plas, Henk C.; Vonk, C. R.; Davelaar, E.; Ribot, S. A. (Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.). *Tetrahedron*, 45(12), 3889-96 (English) 1989. CODEN: TETRAB. ISSN: 0040-4020.

GI

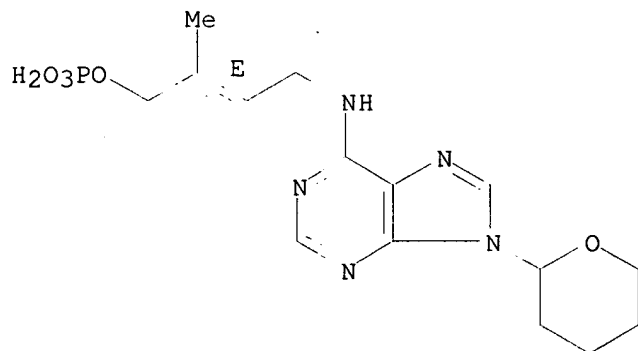


AB Phosphitylation of the allylic hydroxy group in 9-tetrahydropyranyl trans-zeatin (I, R = H) with salicyl chlorophosphite gives the allyl phosphonate I [R = P(O)(OH)H], which can be readily converted into I [R =

P(S)(OH)2, P(O)(OMe)(OH), P(O)(OH)2]. After cleavage of the tetrahydropyranyl group under mild acidic conditions, allylic phosphate derivs. of trans-zeatin are obtained.

L5 ANSWER 85 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 124031-40-9 REGISTRY
CN 2-Buten-1-ol, 2-methyl-4-[[9-(tetrahydro-2H-pyran-2-yl)-9H-purin-6-yl]amino]-, dihydrogen phosphate (ester), disodium salt, (E)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C15 H22 N5 O5 P . 2 Na
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)
CRN (115845-93-7)

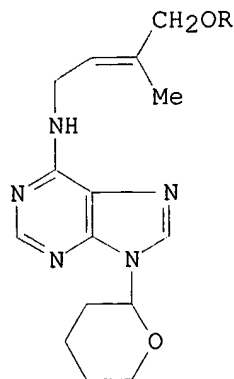
Double bond geometry as shown.



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 112:7250 The synthesis of allylic phosphate derivatives of trans zeatin. Shadid, Belal; Van der Plas, Henk C.; Vonk, C. R.; Davelaar, E.; Ribot, S. A. (Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.). Tetrahedron, 45(12), 3889-96 (English) 1989. CODEN: TETRAB. ISSN: 0040-4020.

GI



AB Phosphitylation of the allylic hydroxy group in 9-tetrahydropyranyl trans-zeatin (I, R = H) with salicyl chlorophosphite gives the allyl phosphonate I [R = P(O)(OH)H], which can be readily converted into I [R = P(S)(OH)2, P(O)(OMe)(OH), P(O)(OH)2]. After cleavage of the tetrahydropyranyl group under mild acidic conditions, allylic phosphate derivs. of trans-zeatin are obtained.

L5 ANSWER 86 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 124031-39-6 REGISTRY

CN Phosphorous acid, 2-methyl-4-[[9-(tetrahydro-2H-pyran-2-yl)-9H-purin-6-yl]amino]-2-butenyl bis(trimethylsilyl) ester, (E)- (9CI) (CA INDEX NAME)

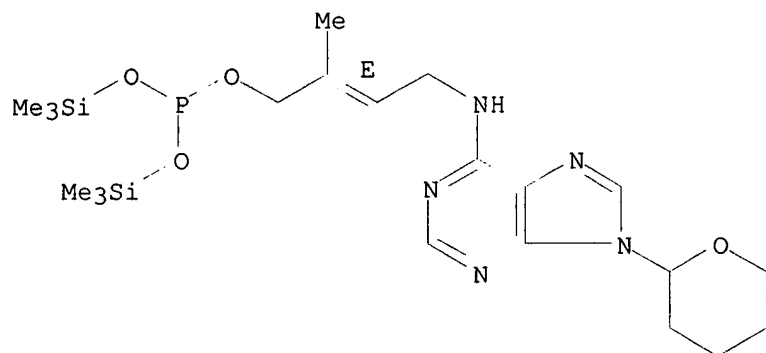
FS STEREOSEARCH

MF C21 H38 N5 O4 P Si2

SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

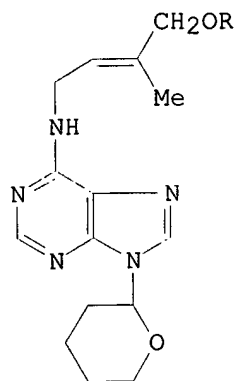
1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 112:7250 The synthesis of allylic phosphate derivatives of trans zeatin. Shadid, Belal; Van der Plas, Henk C.; Vonk, C. R.; Davelaar, E.; Ribot, S. A. (Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.). Tetrahedron, 45(12), 3889-96 (English) 1989.

Searched by: Mary Hale 308-4258 CM-1 1E01

GI



I

AB Phosphitylation of the allylic hydroxy group in 9-tetrahydropyranyl trans-zeatin (I, R = H) with salicyl chlorophosphite gives the allyl phosphonate I [R = P(O)(OH)H], which can be readily converted into I [R = P(S)(OH)2, P(O)(OMe)(OH), P(O)(OH)2]. After cleavage of the tetrahydropyranyl group under mild acidic conditions, allylic phosphate derivs. of trans-zeatin are obtained.

L5 ANSWER 87 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 124031-38-5 REGISTRY

CN Phosphonic acid, mono[2-methyl-4-[[9-(tetrahydro-2H-pyran-2-yl)-9H-purin-6-yl]amino]-2-butenyl] ester, disodium salt, (E)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C15 H22 N5 O4 P . 2 Na

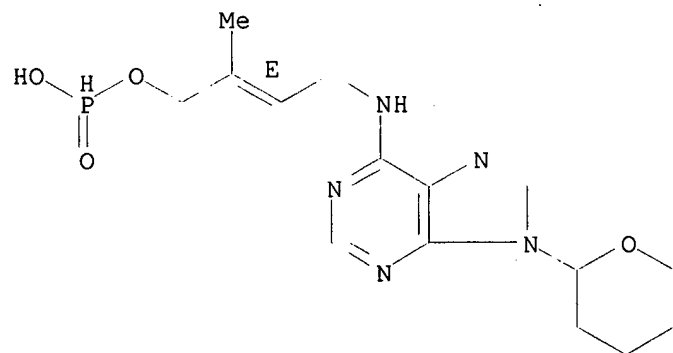
SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT

(*File contains numerically searchable property data)

CRN (115845-92-6)

Double bond geometry as shown.



2 Na

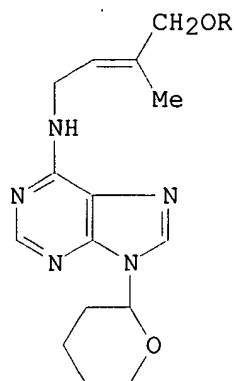
1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

Searched by: Mary Hale 308-4258 CM-1 1E01

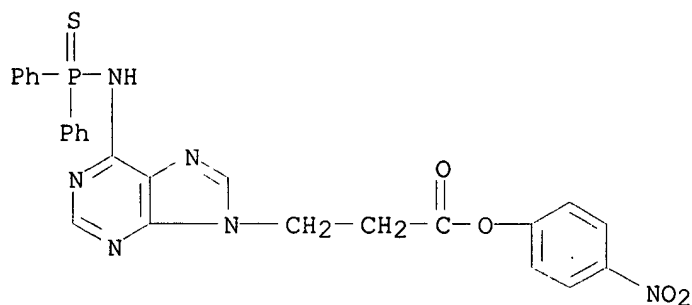
REFERENCE 1: 112:7250 The synthesis of allylic phosphate derivatives of trans zeatin. Shadid, Belal; Van der Plas, Henk C.; Vonk, C. R.; Davelaar, E.; Ribot, S. A. (Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.). Tetrahedron, 45(12), 3889-96 (English) 1989. CODEN: TETRAB. ISSN: 0040-4020.

GI



AB Phosphitylation of the allylic hydroxy group in 9-tetrahydropyranyl trans-zeatin (I, R = H) with salicyl chlorophosphite gives the allyl phosphonate I [R = P(O)(OH)H], which can be readily converted into I [R = P(S)(OH)2, P(O)(OMe)(OH), P(O)(OH)2]. After cleavage of the tetrahydropyranyl group under mild acidic conditions, allylic phosphate derivs. of trans-zeatin are obtained.

L5 ANSWER 88 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 123549-43-9 REGISTRY
 CN 9H-Purine-9-propanoic acid, 6-[(diphenylphosphinothioyl)amino]-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C26 H21 N6 O4 P S
 SR CA
 LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

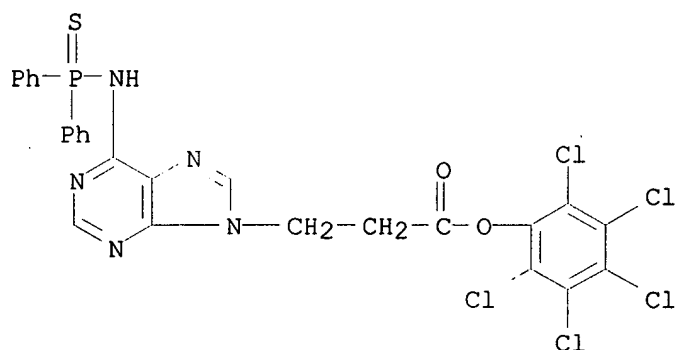
1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

Searched by: Mary Hale 308-4258 CM-1 1E01

REFERENCE 1: 111:195537 Functional monomers and polymers. CLIV.
 Application of nucleic acid base containing polymers to high-performance liquid chromatography. Nagae, Suguru; Suda, Yasuo; Inaki, Yoshiaki; Takemoto, Kiichi (Fac. Eng., Osaka Univ., Suita, 565, Japan). J. Polym. Sci., Part A: Polym. Chem., 27(8), 2593-609 (English) 1989. CODEN: JPACEC. ISSN: 0887-624X.

AB Poly(L-lysine) derivs. contg. pendant nucleic acid bases, such as thymine or adenine, were bonded successfully to 3-aminopropylsilanized silica and silica gel. These resins were useful as the column of HPLC for the selective sepn. of oligoethylenimine derivs. having pendant thymine or adenine bases.

L5 ANSWER 89 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 119225-19-3 REGISTRY
 CN 9H-Purine-9-propanoic acid, 6-[(diphenylphosphinothioyl)amino]-, pentachlorophenyl ester (9CI) (CA INDEX NAME)
 MF C26 H17 Cl5 N5 O2 P S
 SR CA
 LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

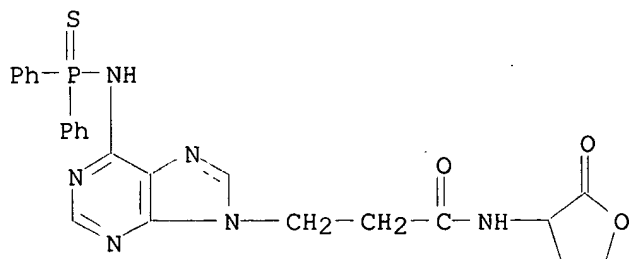
1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 110:95944 Functional monomers and polymers. CLXXII. Synthesis and interaction studies on water-soluble nucleic acid analogs: poly(ethylenimine) derivatives containing thymine and adenine. Wada, Takehiko; Inaki, Yoshiaki; Takemoto, Kiichi (Fac. Eng., Osaka Univ., Suita, 565, Japan). Polym. J. (Tokyo), 20(11), 1059-68 (English) 1988. CODEN: POLJB8. ISSN: 0032-3896.

AB Water-sol. nucleic acid analogs were prep'd. by grafting adenine and thymine derivs. with homoserine onto polyethylenimine. The analogs formed complementary polymer complexes with each other and with polynucleotides. The interactions were studied between these polymers, and with polyuridylic acid and polyadenylic acid in water.

L5 ANSWER 90 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 119225-18-2 REGISTRY
 CN 9H-Purine-9-propanamide, 6-[(diphenylphosphinothioyl)amino]-N-(tetrahydro-2-oxo-3-furanyl)- (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN 9H-Purine-9-propanamide, 6-[(diphenylphosphinothioyl)amino]-N-(tetrahydro-2-oxo-3-furanyl)-, (.-.-.)-
 FS 3D CONCORD

MF C24 H23 N6 O3 P S
 SR CA
 LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

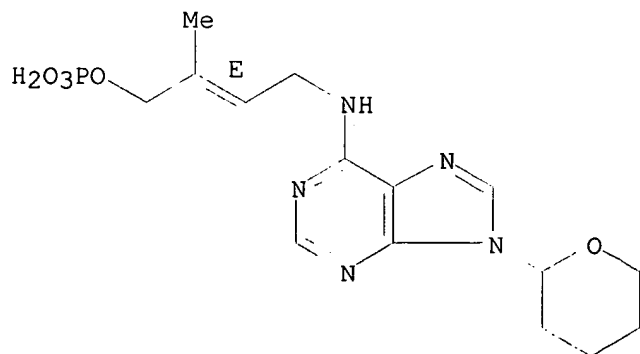
1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 110:95944 Functional monomers and polymers. CLXXII. Synthesis and interaction studies on water-soluble nucleic acid analogs: poly(ethylenimine) derivatives containing thymine and adenine. Wada, Takehiko; Inaki, Yoshiaki; Takemoto, Kiichi (Fac. Eng., Osaka Univ., Suita, 565, Japan). Polym. J. (Tokyo), 20(11), 1059-68 (English) 1988. CODEN: POLJB8. ISSN: 0032-3896.

AB Water-sol. nucleic acid analogs were prep'd. by grafting adenine and thymine derivs. with homoserine onto polyethylenimine. The analogs formed complementary polymer complexes with each other and with polynucleotides. The interactions were studied between these polymers, and with polyuridylic acid and polyadenylic acid in water.

L5 ANSWER 91 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 115845-93-7 REGISTRY
 CN 2-Buten-1-ol, 2-methyl-4-[[9-(tetrahydro-2H-pyran-2-yl)-9H-purin-6-yl]amino]-, dihydrogen phosphate (ester), (E)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C15 H22 N5 O5 P
 CI COM
 SR CA
 LC STN Files: CA, CAPLUS, CASREACT

Double bond geometry as shown.



Searched by: Mary Hale 308-4258 CM-1 1E01

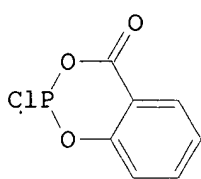
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)

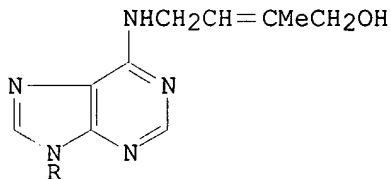
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 109:93147 Phosphorylation of allylic hydroxy groups via phosphite intermediates. Shadid, B. R.; Van der Plas, H. C.; De Vroom, E.; Van der Marel, G. A.; Van Boom, J. H. (Org. Chem. Lab., Agric. Univ., Wageningen, 6703 BC, Neth.). Recl. Trav. Chim. Pays-Bas, 106(9), 509-11 (English) 1987. CODEN: RTCPA3. ISSN: 0165-0513.

GI



I



II

AB Reaction of an allylic hydroxy group in $RCH_2CH:CH_2CMe_2OH$ (R = phthalimide) with salicylchlorophosphite I gives an allyl 1-H-phosphonate monoester, which can be readily hydrolyzed, silylated, and then oxidized to the corresponding phosphate monoester $RCH_2CH:CH_2CMe_2OP(O)(OH)_2$. Application of this phosphite tri-ester approach was further demonstrated in the prepn. of 1-H-phosphonate and phosphate monoesters of N-protected trans-zeatin II (R = tetrahydropyranyl).

L5 ANSWER 92 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 115845-92-6 REGISTRY

CN Phosphonic acid, mono[2-methyl-4-[[9-(tetrahydro-2H-pyran-2-yl)-9H-purin-6-yl]amino]-2-butenyl] ester, (E)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C15 H22 N5 O4 P

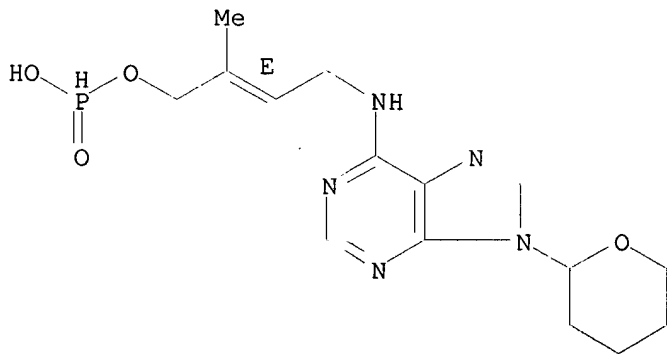
CI COM

SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT

(*File contains numerically searchable property data)

Double bond geometry as shown.



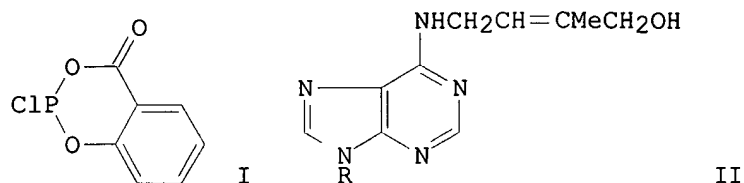
1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

Searched by: Mary Hale 308-4258 CM-1 1E01

REFERENCE 1: 109:93147 Phosphorylation of allylic hydroxy groups via phosphite intermediates. Shadid, B. R.; Van der Plas, H. C.; De Vroom, E.; Van der Marel, G. A.; Van Boom, J. H. (Org. Chem. Lab., Agric. Univ., Wageningen, 6703 BC, Neth.). Recl. Trav. Chim. Pays-Bas, 106(9), 509-11 (English) 1987. CODEN: RTCPA3. ISSN: 0165-0513.

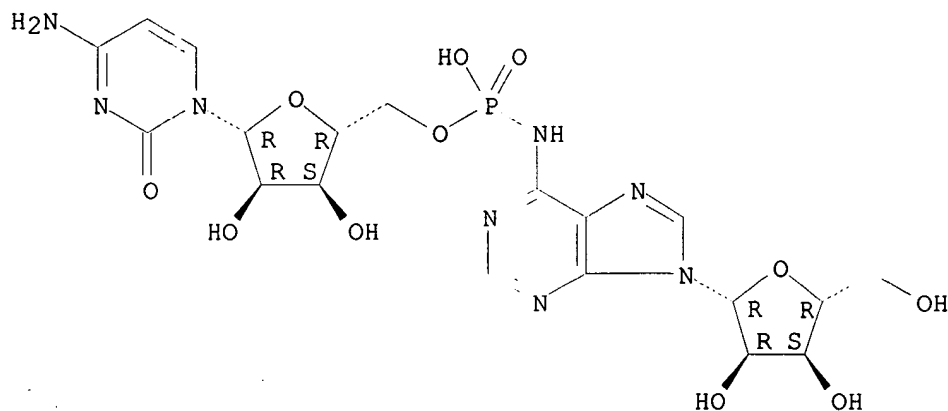
GI



AB Reaction of an allylic hydroxy group in $RCH_2CH:CHMeCH_2OH$ (R = phthalimide) with salicylchlorophosphite I gives an allyl 1-H-phosphonate monoester, which can be readily hydrolyzed, silylated, and then oxidized to the corresponding phosphate monoester $RCH_2CH:CHMeCH_2OP(O)(OH)_2$. Application of this phosphite tri-ester approach was further demonstrated in the prepn. of 1-H-phosphonate and phosphate monoesters of N-protected trans-zeatin II (R = tetrahydropyranyl).

L5 ANSWER 93 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 113729-33-2 REGISTRY
 CN Adenosine, N-5'-cytidyl- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C19 H25 N8 O11 P
 SR CA
 LC STN Files: CA, CAPLUS

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 108:150897 Characteristics of ion evaporation ionization in thermospray high performance liquid chromatography/mass spectrometry.

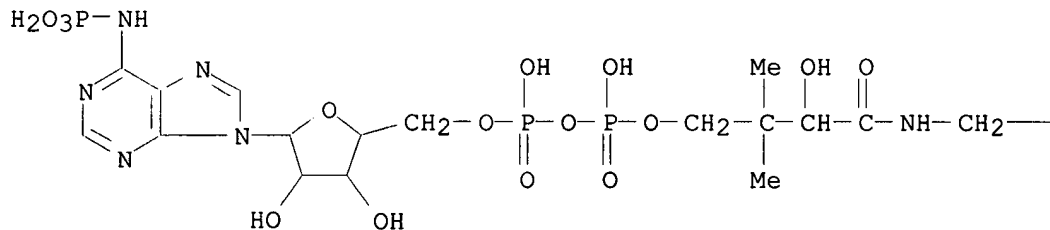
Searched by: Mary Hale 308-4258 CM-1 1E01

Voyksner, Robert D. (Research Triangle Inst., Research Triangle Park, NC, 27709, USA). Org. Mass Spectrom., 22(8), 513-18 (English) 1987. CODEN: ORMSBG. ISSN: 0030-493X.

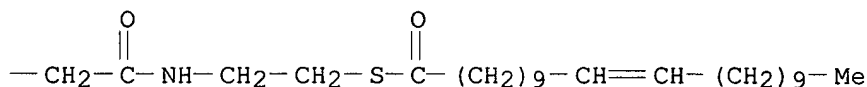
AB Thermospray ion evapn./mass spectrometry in the absence of buffer or auxiliary ionization techniques can prove useful in detecting org. compds. The ion evapn. process appears to be dependent on the type and relative amt. of ionic species in soln. The best sensitivity was obtained at low pH for fully protonated species. The $[M + H]^+$ and $[M + Na]^+$ ion intensities varied directly with soln. acid and salt concn., resp. This dependence enabled the calcn. of $pK'a$ values from thermospray data. Alkali metal adduct ions were favored at a pH where the analyte was ionized in soln. The adduct ions were formed with most alkali metals and the intensity increased with the stability of the ionic complex ($Li > Na > K > Rb > Cs$). The kinetics for the metal adduct ion were different from the $[M + H]^+$ ion formation. Possibly the formation of the $[M + H]^+$ ions occurred by gas-phase reaction based on proton affinities while the metal adducts were derived from desolvated ionic complexes. Ion evapn. spectra without ammonium acetate resembled the type of spectra acquired from desorption ionization techniques (fast atom bombardment). It appears that ion evapn. without buffer is dependent on soln. chem. The addn. of ammonium acetate reduced soln. phase dependence, so the spectra were not changed by the pH.

L5 ANSWER 94 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 111846-63-0 REGISTRY
 CN Coenzyme A, S-11-docosenoate (9CI) (CA INDEX NAME)
 MF C43 H76 N7 O17 P3 S
 SR CA
 LC STN Files: CA, CAPLUS

PAGE 1-A



PAGE 1-B



1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

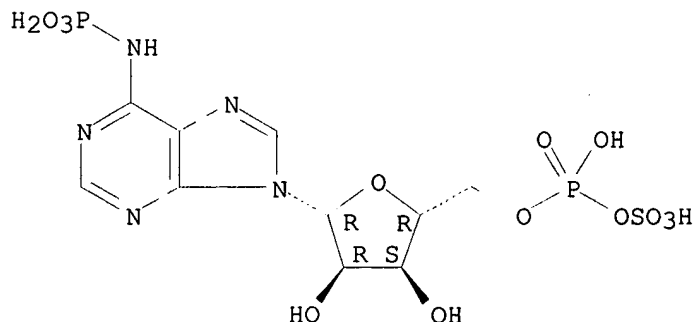
REFERENCE 1: 108:17885 Peroxisomal .beta.-oxidation of long-chain fatty acids possessing different extents of unsaturation. Hovik, Rolf; Osmundsen, Harald (Dent. Sch., Univ. Oslo, Oslo, 0316, Norway). Biochem. J., 247(3), 531-5 (English) 1987. CODEN: BIJOAK. ISSN: 0306-3275.
 AB Rates of peroxisomal .beta.-oxidn. were measured as fatty acyl-CoA-dependent NAD redn. in solubilized peroxisomal fractions isolated from livers of rats treated with clofibrate. Medium- to long-chain satd.

Searched by: Mary Hale 308-4258 CM-1 1E01

fatty acyl-CoA esters as well as long-chain polyunsatd. fatty acyl-CoA esters were used as substrates. Peroxisomal .beta.-oxidn. shows optimal specificity towards long-chain polyunsatd. acyl-CoA esters. Eicosa-8,11,14-trienoyl-CoA, eicosa-11,14,17-trienoyl-CoA, and docosa-7,10,13,16-tetraenoyl-CoA all gave Vmax values of .apprx.150% of that obtained with palmitoyl-CoA. The Km values obtained with these fatty acyl-CoA esters were 17, 13, and 22 .mu.M, resp., which are in the same range as the value for palmitoyl-CoA (13.8 .mu.M). Myristoyl-CoA gave the highest Vmax (110% of the palmitoyl-CoA value) of the satd. fatty acyl-CoAs tested. Substrate inhibition was obsd., with the acyl-CoA esters giving Vmax values >50% of that given by palmitoyl-CoA.

L5 ANSWER 95 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 109434-21-1 REGISTRY
 CN Sulfuric acid, 5'-anhydride with N-phosphono-5'-adenylic acid, lithium salt (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C10 H15 N5 O13 P2 S . x Li
 SR CAS Registry Services

Absolute stereochemistry.



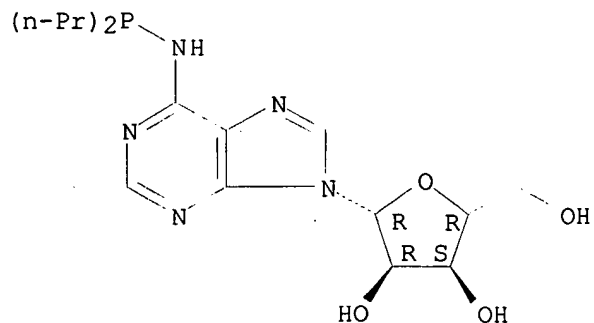
● x Li

L5 ANSWER 96 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 101837-90-5 REGISTRY
 CN Phosphinous amide, N-[9-(O-isopropylidene-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-P,P-dipropyl-, dipropylphosphinite (7CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C25 H43 N5 O4 P2
 CI IDS
 SR CAOLD
 LC STN Files: CAOLD

CM 1

CRN 101837-89-2
 CMF C16 H26 N5 O4 P

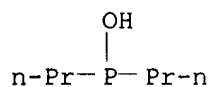
Absolute stereochemistry.



CM 2

CRN 66193-26-8

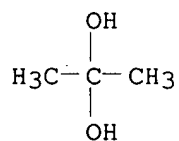
CMF C6 H15 O P



CM 3

CRN 558-18-9

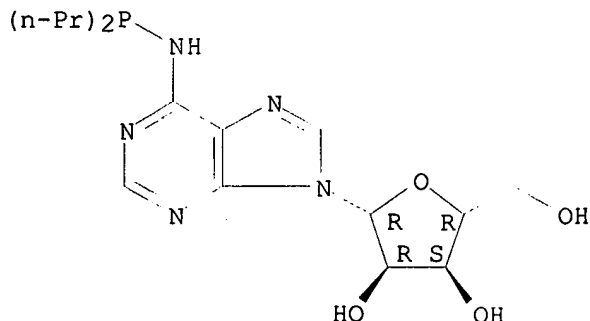
CMF C3 H8 O2



1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L5 ANSWER 97 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 101837-89-2 REGISTRY
 CN Adenosine, N-(dipropylphosphino)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C16 H26 N5 O4 P
 CI COM
 SR CAOLD

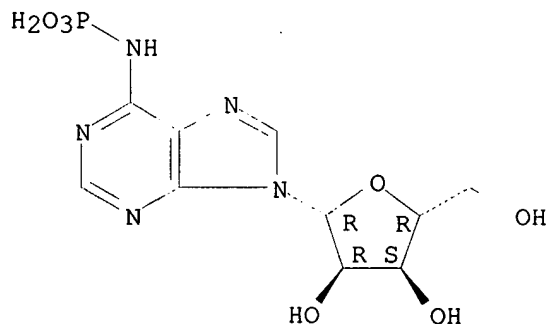
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 98 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 83305-95-7 REGISTRY
 CN Phosphoramidic acid, (9-.beta.-D-ribofuranosyl-9H-purin-6-yl)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C10 H14 N5 O7 P
 CI COM
 LC STN Files: BEILSTEIN*, CA, CAPLUS, MEDLINE
 (*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
 2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 119:49805 Synthesis and properties of adenosine 6-N-phosphoramidate. Wada, Takeshi; Moriguchi, Tomohisa; Sekine, Mitsuo (Fac. Biosci. Biotechnol., Tokyo Inst. Technol., Tokohama, 227, Japan). Nucleic Acids Symp. Ser., 27(Nineteenth Symposium on Nucleic Acids Chemistry, 1992), 93-4 (English) 1992. CODEN: NACSD8. ISSN: 0261-3166.
 AB A symposium report of a new class of phosphorylated nucleosides, e.g. adenosine 6-N-phosphoramidate (6-N-AMP) and its derivs. which were synthesized and their properties investigated.

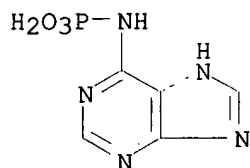
REFERENCE 2: 97:158438 Physicochemical studies on phosphorylation. Ghosh, Guru Prasanna (Sheila Dhar Inst. Soil Sci., Allahabad Univ., Allahabad,

Searched by: Mary Hale 308-4258 CM-1 1E01

211 002, India). J. Indian Chem. Soc., 59(4), 599-602 (English) 1982.
CODEN: JICSAH. ISSN: 0019-4522.

AB Cryoscopic, ebullioscopic, conductometric, and pH detns. were carried out of orthophosphoric acid alone and mixed with adenine, creatine, glycine, asparagine, methionine, glutamic acid, urea, glucose, and sucrose. The results indicate that monomol. complexes are formed by the interaction of phosphoric acid with purines, creatine, and amino acids in the absence of enzymes and that these complexes are stable, even in boiling soln.

L5 ANSWER 99 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 83305-93-5 REGISTRY
CN Phosphoramidic acid, 1H-purin-6-yl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C5 H6 N5 O3 P
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

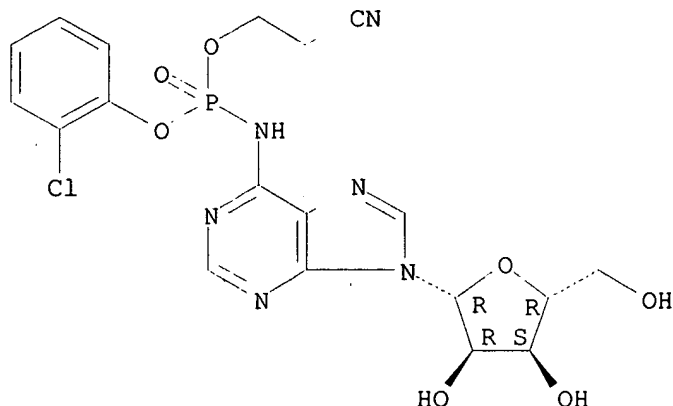
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 97:158438 Physicochemical studies on phosphorylation. Ghosh, Guru Prasanna (Sheila Dhar Inst. Soil Sci., Allahabad Univ., Allahabad, 211 002, India). J. Indian Chem. Soc., 59(4), 599-602 (English) 1982.
CODEN: JICSAH. ISSN: 0019-4522.

AB Cryoscopic, ebullioscopic, conductometric, and pH detns. were carried out of orthophosphoric acid alone and mixed with adenine, creatine, glycine, asparagine, methionine, glutamic acid, urea, glucose, and sucrose. The results indicate that monomol. complexes are formed by the interaction of phosphoric acid with purines, creatine, and amino acids in the absence of enzymes and that these complexes are stable, even in boiling soln.

L5 ANSWER 100 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 78111-44-1 REGISTRY
CN Adenosine, N-[(2-chlorophenoxy)(2-cyanoethoxy)phosphinyl]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C19 H20 Cl N6 O7 P
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

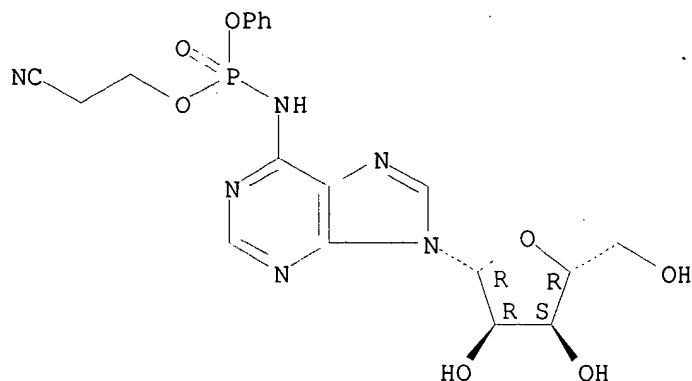
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 95:25488 Nucleotides. XIII. Phosphorylations of adenosine and 2'-deoxyadenosine by phosphorochloridates. Charubala, Ramamurthy; Pfleiderer, Wolfgang (Fak. Chem., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger.). Heterocycles, 15(2), 761-76 (English) 1981. CODEN: HTCYAM. ISSN: 0385-5414.

AB Phosphorylations of adenosine and 2'-deoxyadenosine by various phosphorylating agents, e.g., (PhO)₂P(O)Cl, were achieved at positions 3', 5', and N-6 using appropriate starting materials for unambiguous synthesis. There is a difference in the reactivity of the different functions in these mols. with a preference of the 5'-OH followed by 6-NH₂ and then 3'-OH in the 3rd place. UV and CD spectral data and pK_a values of various adenosine and 2'-deoxyadenosine phosphotriesters prep'd. are given.

L5 ANSWER 101 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 78111-43-0 REGISTRY
CN Adenosine, N-[(2-cyanoethoxy)phenoxyphosphinyl]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C19 H21 N6 O7 P
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.

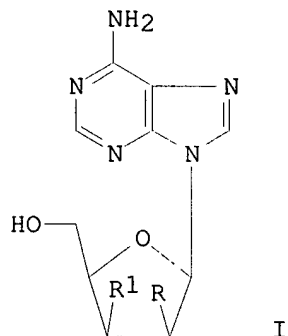


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 120:271041 Nucleic acid related compounds. 81. Syntheses of 9-(3-deoxy-.beta.-D-threo-pentofuranosyl)adenine, the core nucleoside of the extraordinarily selective antibiotic agrocin 84, and simplified structural component analogs. Vinayak, Ravi; Hansske, Fritz; Robins, Morris J. (Dep. Chem., Univ. Alberta, Edmonton, AB, Can.). J. Heterocycl. Chem., 30(5), 1181-9 (English) 1993. CODEN: JHTCAD. ISSN: 0022-152X.

GI



AB Alternative syntheses of (deoxy-.beta.-D-threo-pentofuranosyl)adenine I (R = OH, R1 = H) (II), the core nucleoside of agrocin 84 and its 2'-deoxy threo isomer I (R = H, R1 = OH) (III) were devised: (1) direct conversion of 9-(.beta.-D-arabinofuranosyl)adenine into 9-(2,3-anhydro-.beta.-D-lyxofuranosyl)adenine and regioselective opening of its oxirane ring with sodium borohydride to give II and III (.apprx.7.5:1); (2) treatment of adenosine with sodium hydride and 2,4,6-triisopropylbenzenesulfonyl chloride, and subjection of the resulting 2'(3')-sulfonates to the reductive [1,2]-hydride shift rearrangement with lithium triethylborohydride to give II and III (.apprx.2:1); and (3) subjection of the phenoxythiocarbonyl esters of 9-[2(3),5-bis-O-(tert-butylidimethylsilyl)-.beta.-D-arabinofuranosyl]adenine to Barton deoxygenation, and deprotection to give II and 2'-deoxyadenosine (.apprx.5:1). Methods (2) and (3) gave lower yields. Syntheses of simplified 6-N- and 5'-O-adenosine phosphoramidate model compds. were

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explored to examine potential access to such features in the structure proposed for agrocin 84.

REFERENCE 2: 95:25488 Nucleotides. XIII. Phosphorylations of adenosine and 2'-deoxyadenosine by phosphorochloridates. Charubala, Ramamurthy; Pfleiderer, Wolfgang (Fak. Chem., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger.). Heterocycles, 15(2), 761-76 (English) 1981. CODEN: HTCYAM. ISSN: 0385-5414.

AB Phosphorylations of adenosine and 2'-deoxyadenosine by various phosphorylating agents, e.g., (PhO)₂P(O)Cl, were achieved at positions 3',5', and N-6 using appropriate starting materials for unambiguous synthesis. There is a difference in the reactivity of the different functions in these mols. with a preference of the 5'-OH followed by 6-NH₂ and then 3'-OH in the 3rd place. UV and CD spectral data and pK_a values of various adenosine and 2'-deoxyadenosine phosphotriesters prep'd. are given.

L5 ANSWER 102 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 78111-42-9 REGISTRY

CN Adenosine, N-[bis(2-chlorophenoxy)phosphinyl]- (9CI) (CA INDEX NAME)

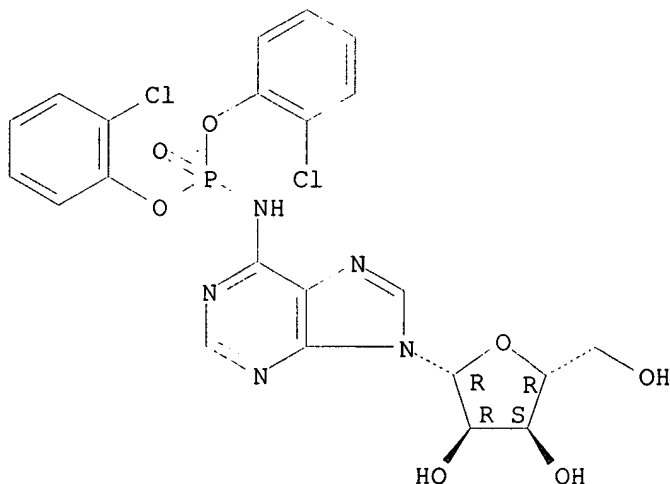
FS STEREOSEARCH

MF C22 H20 Cl2 N5 O7 P

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 95:25488 Nucleotides. XIII. Phosphorylations of adenosine and 2'-deoxyadenosine by phosphorochloridates. Charubala, Ramamurthy; Pfleiderer, Wolfgang (Fak. Chem., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger.). Heterocycles, 15(2), 761-76 (English) 1981. CODEN: HTCYAM. ISSN: 0385-5414.

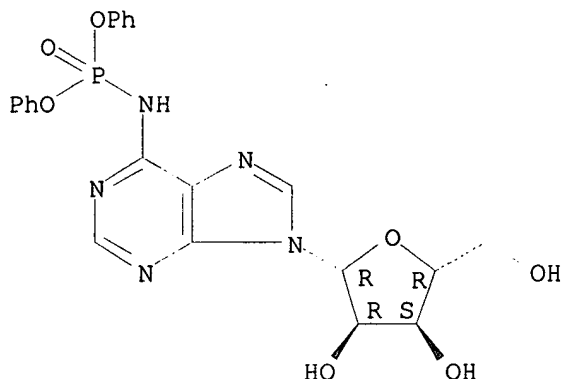
AB Phosphorylations of adenosine and 2'-deoxyadenosine by various phosphorylating agents, e.g., (PhO)₂P(O)Cl, were achieved at positions 3',5', and N-6 using appropriate starting materials for unambiguous synthesis. There is a difference in the reactivity of the different functions in these mols. with a preference of the 5'-OH followed by 6-NH₂

Searched by: Mary Hale 308-4258 CM-1 1E01

and then 3'-OH in the 3rd place. UV and CD spectral data and pKa values of various adenosine and 2'-deoxyadenosine phosphotriesters prepd. are given.

L5 ANSWER 103 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 78111-41-8 REGISTRY
CN Adenosine, N-(diphenoxyphosphinyl)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C22 H22 N5 O7 P
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

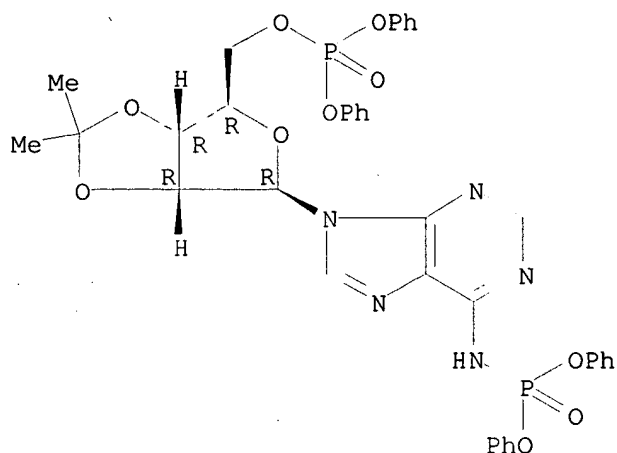
- REFERENCE 1: 96:214695 Vasoactivities of adenosine analogs in trout gill (Salmo gairdneri R.). Colin, Didier A.; Leray, Claude (Lab. Physiol. Comp. Regul., CNRS, Strasbourg, F-67037, Fr.). Biochem. Pharmacol., 30(21), 2971-7 (English) 1981. CODEN: BCPCA6. ISSN: 0006-2952.
- AB Various adenosine analogs, phosphorylated or not, modified at the purine or in the carbohydrate moiety, were tested for their ability to induce a vasoconstriction in the arterio-arterial vascular bed of the trout gill. Structure-activity relations were detd. The results sustained the hypothesis of the presence of specific vascular purinergic receptors in the trout gill.
- REFERENCE 2: 95:25488 Nucleotides. XIII. Phosphorylations of adenosine and 2'-deoxyadenosine by phosphorochloridates. Charubala, Ramamurthy; Pfleiderer, Wolfgang (Fak. Chem., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger.). Heterocycles, 15(2), 761-76 (English) 1981. CODEN: HTCYAM. ISSN: 0385-5414.
- AB Phosphorylations of adenosine and 2'-deoxyadenosine by various phosphorylating agents, e.g., (PhO)₂P(O)Cl, were achieved at positions 3', 5', and N-6 using appropriate starting materials for unambiguous synthesis. There is a difference in the reactivity of the different functions in these mols. with a preference of the 5'-OH followed by 6-NH₂ and then 3'-OH in the 3rd place. UV and CD spectral data and pKa values of various adenosine and 2'-deoxyadenosine phosphotriesters prepd. are given.

L5 ANSWER 104 OF 140 REGISTRY COPYRIGHT 2002 ACS

Searched by: Mary Hale 308-4258 CM-1 1E01

RN 78111-40-7 REGISTRY
 CN 5'-Adenylic acid, N-(diphenoxyphosphinyl)-2',3'-O-(1-methylethylidene)-, diphenyl ester (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Furo[3,4-d]-1,3-dioxole, 5'-adenylic acid deriv.
 FS STEREOSEARCH
 MF C37 H35 N5 O10 P2
 LC STN Files: BEILSTEIN*, CA, CAPLUS
 (*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

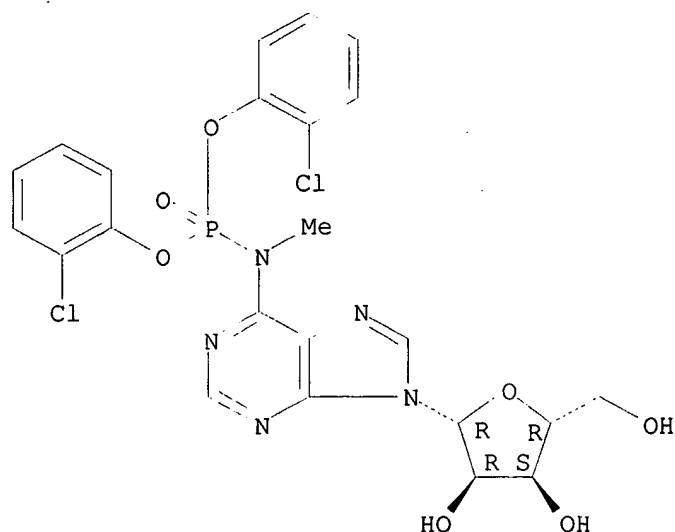
REFERENCE 1: 95:25488 Nucleotides. XIII. Phosphorylations of adenosine and 2'-deoxyadenosine by phosphorochloridates. Charubala, Ramamurthy; Pfleiderer, Wolfgang (Fak. Chem., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger.). Heterocycles, 15(2), 761-76 (English) 1981. CODEN: HTCYAM. ISSN: 0385-5414.

AB Phosphorylations of adenosine and 2'-deoxyadenosine by various phosphorylating agents, e.g., (PhO)2P(O)Cl, were achieved at positions 3',5', and N-6 using appropriate starting materials for unambiguous synthesis. There is a difference in the reactivity of the different functions in these mols. with a preference of the 5'-OH followed by 6-NH2 and then 3'-OH in the 3rd place. UV and CD spectral data and pKa values of various adenosine and 2'-deoxyadenosine phosphotriesters prep'd. are given.

L5 ANSWER 105 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 78098-71-2 REGISTRY
 CN Phosphoramidic acid, methyl(9-.beta.-D-ribofuranosyl-9H-purin-6-yl)-, bis(2-chlorophenyl) ester (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C23 H22 Cl2 N5 O7 P
 LC STN Files: BEILSTEIN*, CA, CAPLUS
 (*File contains numerically searchable property data)

Absolute stereochemistry.

Searched by: Mary Hale 308-4258 CM-1 1E01



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 95:25488 Nucleotides. XIII. Phosphorylations of adenosine and 2'-deoxyadenosine by phosphorochloridates. Charubala, Ramamurthy; Pfleiderer, Wolfgang (Fak. Chem., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger.). Heterocycles, 15(2), 761-76 (English) 1981. CODEN: HTCYAM. ISSN: 0385-5414.

AB Phosphorylations of adenosine and 2'-deoxyadenosine by various phosphorylating agents, e.g., (PhO)₂P(O)Cl, were achieved at positions 3', 5', and N-6 using appropriate starting materials for unambiguous synthesis. There is a difference in the reactivity of the different functions in these mols. with a preference of the 5'-OH followed by 6-NH₂ and then 3'-OH in the 3rd place. UV and CD spectral data and pK_a values of various adenosine and 2'-deoxyadenosine phosphotriesters prep'd. are given.

L5 ANSWER 106 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 78098-70-1 REGISTRY

CN Phosphoramidic acid, [9-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, 2-chlorophenyl 2-cyanoethyl ester (9CI) (CA INDEX NAME)

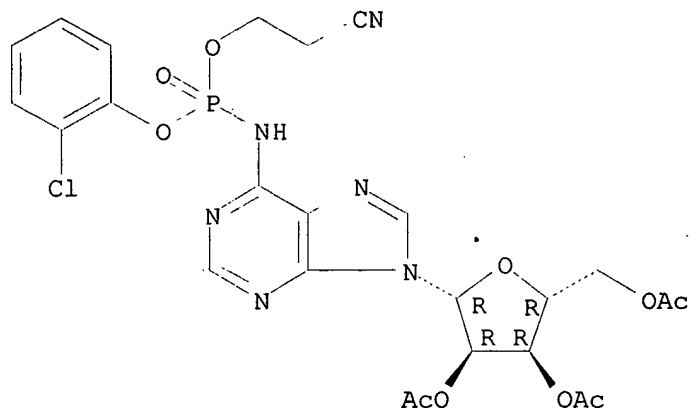
FS STEREOSEARCH

MF C25 H26 Cl N6 O10 P

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 95:25488 Nucleotides. XIII. Phosphorylations of adenosine and 2'-deoxyadenosine by phosphorochloridates. Charubala, Ramamurthy; Pfleiderer, Wolfgang (Fak. Chem., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger.). Heterocycles, 15(2), 761-76 (English) 1981. CODEN: HTCYAM. ISSN: '0385-5414.

AB Phosphorylations of adenosine and 2'-deoxyadenosine by various phosphorylating agents, e.g., (PhO)2P(O)Cl, were achieved at positions 3', 5', and N-6 using appropriate starting materials for unambiguous synthesis. There is a difference in the reactivity of the different functions in these mols. with a preference of the 5'-OH followed by 6-NH2 and then 3'-OH in the 3rd place. UV and CD spectral data and pKa values of various adenosine and 2'-deoxyadenosine phosphotriesters prepd. are given.

L5 ANSWER 107 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 78098-69-8 REGISTRY

CN Phosphoramidic acid, [9-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, 2-cyanoethyl phenyl ester (9CI) (CA INDEX NAME)

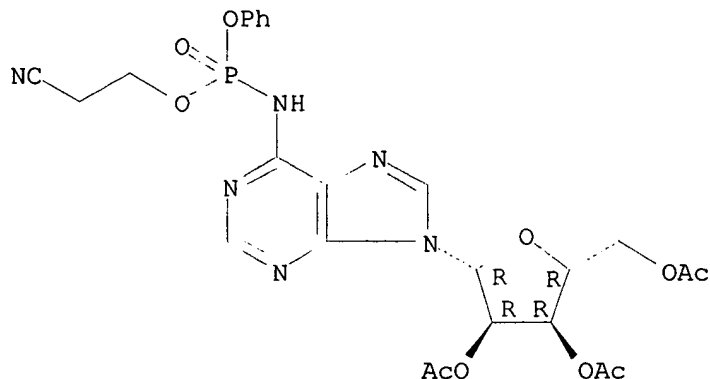
FS STEREOSEARCH

MF C25 H27 N6 O10 P

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

Absolute stereochemistry.

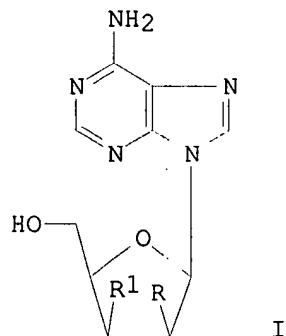


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 120:271041 Nucleic acid related compounds. 81. Syntheses of 9-(3-deoxy-.beta.-D-threo-pentofuranosyl)adenine, the core nucleoside of the extraordinarily selective antibiotic agrocin 84, and simplified structural component analogs. Vinayak, Ravi; Hansske, Fritz; Robins, Morris J. (Dep. Chem., Univ. Alberta, Edmonton, AB, Can.). J. Heterocycl. Chem., 30(5), 1181-9 (English) 1993. CODEN: JHTCAD. ISSN: 0022-152X.

GI



AB Alternative syntheses of (deoxy-.beta.-D-threo-pentofuranosyl)adenine I (R = OH, R1 = H) (II), the core nucleoside of agrocin 84 and its 2'-deoxy threo isomer I (R = H, R1 = OH) (III) were devised: (1) direct conversion of 9-(.beta.-D-arabinofuranosyl)adenine into 9-(2,3-anhydro-.beta.-D-lyxofuranosyl)adenine and regioselective opening of its oxirane ring with sodium borohydride to give II and III (.apprx.7.5:1); (2) treatment of adenosine with sodium hydride and 2,4,6-triisopropylbenzenesulfonyl chloride, and subjection of the resulting 2'(3')-sulfonates to the reductive [1,2]-hydride shift rearrangement with lithium triethylborohydride to give II and III (.apprx.2:1); and (3) subjection of the phenoxythiocarbonyl esters of 9-[2(3),5-bis-O-(tert-butylidimethylsilyl)-.beta.-D-arabinofuranosyl]adenine to Barton deoxygenation, and deprotection to give II and 2'-deoxyadenosine (.apprx.5:1). Methods (2) and (3) gave lower yields. Syntheses of simplified 6-N- and 5'-O-adenosine phosphoramidate model compds. were

explored to examine potential access to such features in the structure proposed for agrocin 84.

REFERENCE 2: 95:25488 Nucleotides. XIII. Phosphorylations of adenosine and 2'-deoxyadenosine by phosphorochloridates. Charubala, Ramamurthy; Pfleiderer, Wolfgang (Fak. Chem., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger.). Heterocycles, 15(2), 761-76 (English) 1981. CODEN: HTCYAM. ISSN: 0385-5414.

AB Phosphorylations of adenosine and 2'-deoxyadenosine by various phosphorylating agents, e.g., (PhO)2P(O)Cl, were achieved at positions 3',5', and N-6 using appropriate starting materials for unambiguous synthesis. There is a difference in the reactivity of the different functions in these mols. with a preference of the 5'-OH followed by 6-NH2 and then 3'-OH in the 3rd place. UV and CD spectral data and pKa values of various adenosine and 2'-deoxyadenosine phosphotriesters prep'd. are given.

L5 ANSWER 108 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 78098-68-7 REGISTRY

CN Phosphoramidic acid, methyl[9-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, bis(2-chlorophenyl) ester (9CI) (CA INDEX NAME)

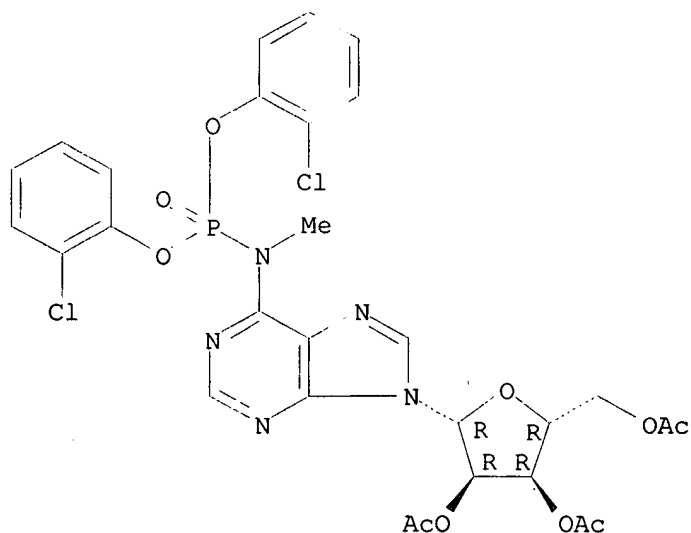
FS STEREOSEARCH

MF C29 H28 Cl2 N5 O10 P

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 95:25488 Nucleotides. XIII. Phosphorylations of adenosine and 2'-deoxyadenosine by phosphorochloridates. Charubala, Ramamurthy; Pfleiderer, Wolfgang (Fak. Chem., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger.). Heterocycles, 15(2), 761-76 (English) 1981. CODEN: HTCYAM. ISSN: 0385-5414.

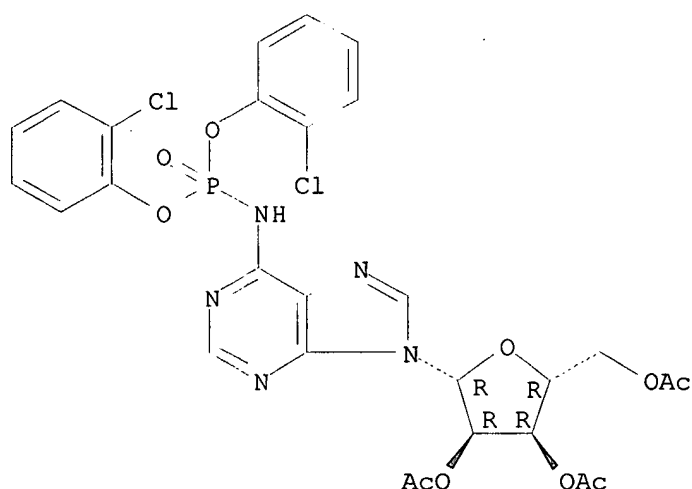
AB Phosphorylations of adenosine and 2'-deoxyadenosine by various phosphorylating agents, e.g., (PhO)2P(O)Cl, were achieved at positions

Searched by: Mary Hale 308-4258 CM-1 1E01

3',5', and N-6 using appropriate starting materials for unambiguous synthesis. There is a difference in the reactivity of the different functions in these mols. with a preference of the 5'-OH followed by 6-NH₂ and then 3'-OH in the 3rd place. UV and CD spectral data and pK_a values of various adenosine and 2'-deoxyadenosine phosphotriesters prepd. are given.

L5 ANSWER 109 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 78098-67-6 REGISTRY
 CN Phosphoramidic acid, [9-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, bis(2-chlorophenyl) ester (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C28 H26 Cl2 N5 O10 P
 LC STN Files: BEILSTEIN*, CA, CAPLUS
 (*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 95:25488 Nucleotides. XIII. Phosphorylations of adenosine and 2'-deoxyadenosine by phosphorochloridates. Charubala, Ramamurthy; Pfleiderer, Wolfgang (Fak. Chem., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger.). Heterocycles, 15(2), 761-76 (English) 1981. CODEN: HTCYAM. ISSN: 0385-5414.

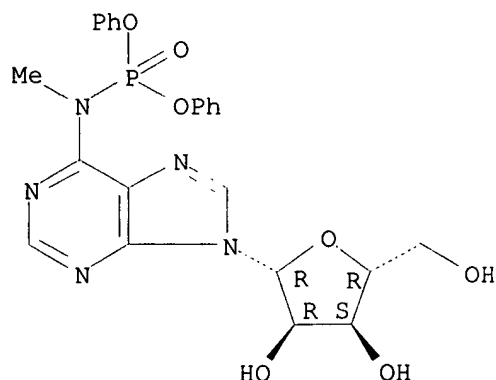
AB Phosphorylations of adenosine and 2'-deoxyadenosine by various phosphorylating agents, e.g., (PhO)₂P(O)Cl, were achieved at positions 3',5', and N-6 using appropriate starting materials for unambiguous synthesis. There is a difference in the reactivity of the different functions in these mols. with a preference of the 5'-OH followed by 6-NH₂ and then 3'-OH in the 3rd place. UV and CD spectral data and pK_a values of various adenosine and 2'-deoxyadenosine phosphotriesters prepd. are given.

L5 ANSWER 110 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 78098-66-5 REGISTRY
 CN Phosphoramidic acid, methyl(9-.beta.-D-ribofuranosyl-9H-purin-6-yl)-, diphenyl ester (9CI) (CA INDEX NAME)
 FS STEREOSEARCH

Searched by: Mary Hale 308-4258 CM-1 1E01

MF C23 H24 N5 O7 P
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 96:214695 Vasoactivities of adenosine analogs in trout gill (Salmo gairdneri R.). Colin, Didier A.; Leray, Claude (Lab. Physiol. Comp. Regul., CNRS, Strasbourg, F-67037, Fr.). Biochem. Pharmacol., 30(21), 2971-7 (English) 1981. CODEN: BCPCA6. ISSN: 0006-2952.

AB Various adenosine analogs, phosphorylated or not, modified at the purine or in the carbohydrate moiety, were tested for their ability to induce a vasoconstriction in the arterio-arterial vascular bed of the trout gill. Structure-activity relations were detd. The results sustained the hypothesis of the presence of specific vascular purinergic receptors in the trout gill.

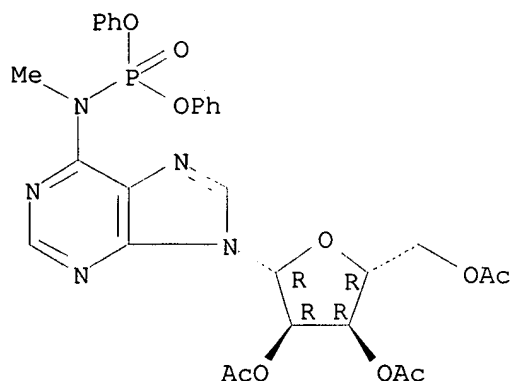
REFERENCE 2: 95:25488 Nucleotides. XIII. Phosphorylations of adenosine and 2'-deoxyadenosine by phosphorochloridates. Charubala, Ramamurthy; Pfeleiderer, Wolfgang (Fak. Chem., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger.). Heterocycles, 15(2), 761-76 (English) 1981. CODEN: HTCYAM. ISSN: 0385-5414.

AB Phosphorylations of adenosine and 2'-deoxyadenosine by various phosphorylating agents, e.g., (PhO)2P(O)Cl, were achieved at positions 3', 5', and N-6 using appropriate starting materials for unambiguous synthesis. There is a difference in the reactivity of the different functions in these mols. with a preference of the 5'-OH followed by 6-NH2 and then 3'-OH in the 3rd place. UV and CD spectral data and pKa values of various adenosine and 2'-deoxyadenosine phosphotriesters prep'd. are given.

L5 ANSWER 111 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 78098-65-4 REGISTRY
CN Phosphoramidic acid, methyl[9-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, diphenyl ester (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C29 H30 N5 O10 P
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Searched by: Mary Hale 308-4258 CM-1 1E01

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 95:25488 Nucleotides. XIII. Phosphorylations of adenosine and 2'-deoxyadenosine by phosphorochloridates. Charubala, Ramamurthy; Pfleiderer, Wolfgang (Fak. Chem., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger.). Heterocycles, 15(2), 761-76 (English) 1981. CODEN: HTCYAM. ISSN: 0385-5414.

AB Phosphorylations of adenosine and 2'-deoxyadenosine by various phosphorylating agents, e.g., (PhO)₂P(O)Cl, were achieved at positions 3', 5', and N-6 using appropriate starting materials for unambiguous synthesis. There is a difference in the reactivity of the different functions in these mols. with a preference of the 5'-OH followed by 6-NH₂ and then 3'-OH in the 3rd place. UV and CD spectral data and pK_a values of various adenosine and 2'-deoxyadenosine phosphotriesters prepd. are given.

L5 ANSWER 112 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 78098-64-3 REGISTRY

CN Phosphoramidic acid, [9-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, diphenyl ester (9CI) (CA INDEX NAME)

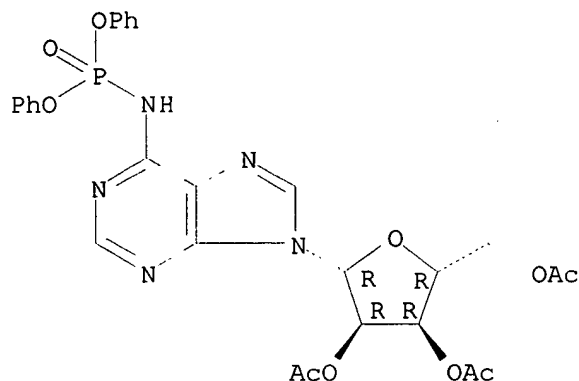
FS STEREOSEARCH

MF C28 H28 N5 O10 P

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

Absolute stereochemistry.



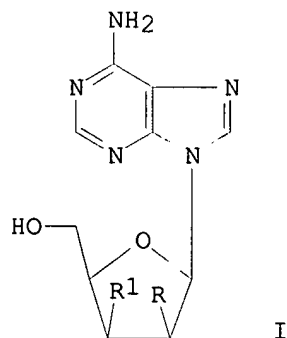
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)

2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 120:271041 Nucleic acid related compounds. 81. Syntheses of 9-(3-deoxy-.beta.-D-threo-pentofuranosyl)adenine, the core nucleoside of the extraordinarily selective antibiotic agrocin 84, and simplified structural component analogs. Vinayak, Ravi; Hansske, Fritz; Robins, Morris J. (Dep. Chem., Univ. Alberta, Edmonton, AB, Can.). J. Heterocycl. Chem., 30(5), 1181-9 (English) 1993. CODEN: JHTCAD. ISSN: 0022-152X.

GI



AB Alternative syntheses of (deoxy-.beta.-D-threo-pentofuranosyl)adenine I (R = OH, R1 = H) (II), the core nucleoside of agrocin 84 and its 2'-deoxy threo isomer I (R = H, R1 = OH) (III) were devised: (1) direct conversion of 9-(.beta.-D-arabinofuranosyl)adenine into 9-(2,3-anhydro-.beta.-D-lyxofuranosyl)adenine and regioselective opening of its oxirane ring with sodium borohydride to give II and III (.apprx.7.5:1); (2) treatment of adenosine with sodium hydride and 2,4,6-triisopropylbenzenesulfonyl chloride, and subjection of the resulting 2'(3')-sulfonates to the reductive [1,2]-hydride shift rearrangement with lithium triethylborohydride to give II and III (.apprx.2:1); and (3) subjection of the phenoxythiocarbonyl esters of 9-[2(3),5-bis-O-(tert-butylidimethylsilyl)-.beta.-D-arabinofuranosyl]adenine to Barton deoxygenation, and deprotection to give II and 2'-deoxyadenosine (.apprx.5:1). Methods (2) and (3) gave lower yields. Syntheses of simplified 6-N- and 5'-O-adenosine phosphoramidate model compds. were

explored to examine potential access to such features in the structure proposed for agrocin 84.

REFERENCE 2: 95:25488 Nucleotides. XIII. Phosphorylations of adenosine and 2'-deoxyadenosine by phosphorochloridates. Charubala, Ramamurthy; Pfleiderer, Wolfgang (Fak. Chem., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger.). Heterocycles, 15(2), 761-76 (English) 1981. CODEN: HTCYAM. ISSN: 0385-5414.

AB Phosphorylations of adenosine and 2'-deoxyadenosine by various phosphorylating agents, e.g., (PhO)₂P(O)Cl, were achieved at positions 3',5', and N-6 using appropriate starting materials for unambiguous synthesis. There is a difference in the reactivity of the different functions in these mols. with a preference of the 5'-OH followed by 6-NH₂ and then 3'-OH in the 3rd place. UV and CD spectral data and pK_a values of various adenosine and 2'-deoxyadenosine phosphotriesters prep'd. are given.

L5 ANSWER 113 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 78098-63-2 REGISTRY

CN Phosphoramidic acid, [9-(3,5-di-O-acetyl-2-deoxy-.beta.-D-erythro-pentofuranosyl)-9H-purin-6-yl]-, diphenyl ester (9CI) (CA INDEX NAME)

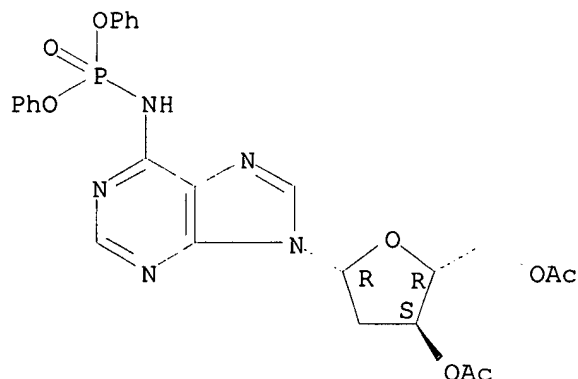
FS STEREOSEARCH

MF C26 H26 N5 O8 P

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 95:25488 Nucleotides. XIII. Phosphorylations of adenosine and 2'-deoxyadenosine by phosphorochloridates. Charubala, Ramamurthy; Pfleiderer, Wolfgang (Fak. Chem., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger.). Heterocycles, 15(2), 761-76 (English) 1981. CODEN: HTCYAM. ISSN: 0385-5414.

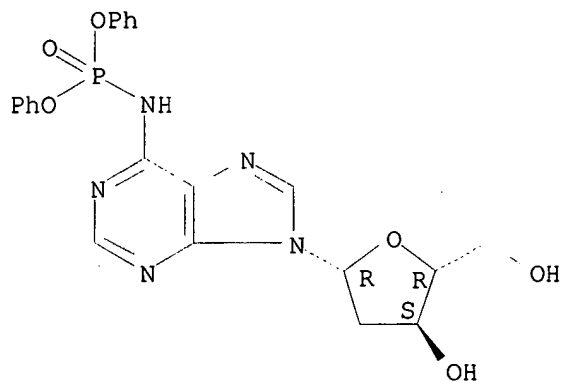
AB Phosphorylations of adenosine and 2'-deoxyadenosine by various phosphorylating agents, e.g., (PhO)₂P(O)Cl, were achieved at positions 3',5', and N-6 using appropriate starting materials for unambiguous synthesis. There is a difference in the reactivity of the different functions in these mols. with a preference of the 5'-OH followed by 6-NH₂ and then 3'-OH in the 3rd place. UV and CD spectral data and pK_a values of various adenosine and 2'-deoxyadenosine phosphotriesters prep'd. are

Searched by: Mary Hale 308-4258 CM-1 1E01

given.

L5 ANSWER 114 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 78098-60-9 REGISTRY
CN Phosphoramidic acid, [9-(2-deoxy-.beta.-D-erythro-pentofuranosyl)-9H-purin-6-yl]-, diphenyl ester (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C22 H22 N5 O6 P
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

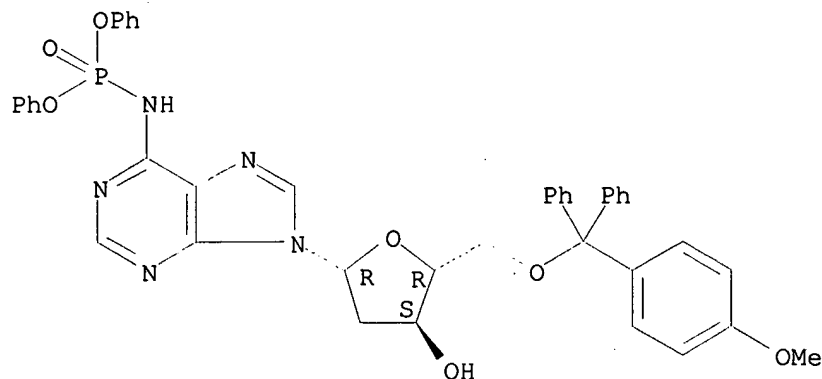
REFERENCE 1: 95:25488 Nucleotides. XIII. Phosphorylations of adenosine and 2'-deoxyadenosine by phosphorochloridates. Charubala, Ramamurthy; Pfleiderer, Wolfgang (Fak. Chem., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger.). Heterocycles, 15(2), 761-76 (English) 1981. CODEN: HTCYAM. ISSN: 0385-5414.

AB Phosphorylations of adenosine and 2'-deoxyadenosine by various phosphorylating agents, e.g., (PhO)2P(O)Cl, were achieved at positions 3', 5', and N-6 using appropriate starting materials for unambiguous synthesis. There is a difference in the reactivity of the different functions in these mols. with a preference of the 5'-OH followed by 6-NH2 and then 3'-OH in the 3rd place. UV and CD spectral data and pKa values of various adenosine and 2'-deoxyadenosine phosphotriesters prep'd. are given.

L5 ANSWER 115 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 78098-58-5 REGISTRY
CN Phosphoramidic acid, [9-[2-deoxy-5-O-[(4-methoxyphenyl)diphenylmethyl]-.beta.-D-erythro-pentofuranosyl]-9H-purin-6-yl]-, diphenyl ester (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C42 H38 N5 O7 P
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.

Searched by: Mary Hale 308-4258 CM-1 1E01



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

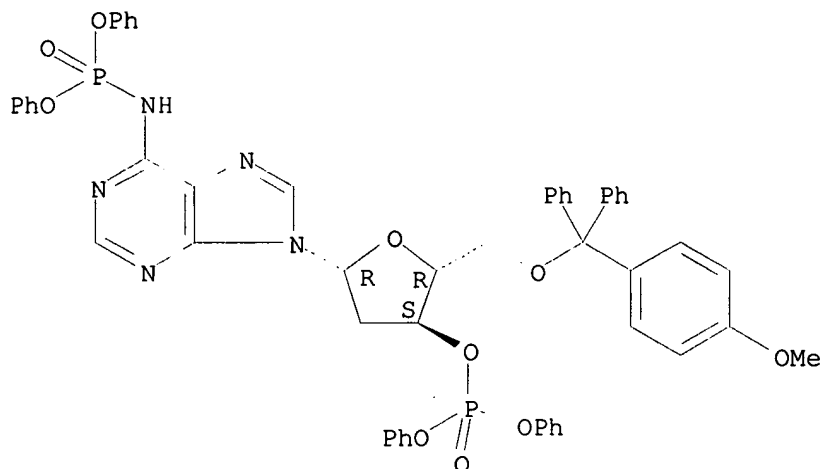
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 95:25488 Nucleotides. XIII. Phosphorylations of adenosine and 2'-deoxyadenosine by phosphorochloridates. Charubala, Ramamurthy; Pfleiderer, Wolfgang (Fak. Chem., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger.). Heterocycles, 15(2), 761-76 (English) 1981. CODEN: HTCYAM. ISSN: 0385-5414.

AB Phosphorylations of adenosine and 2'-deoxyadenosine by various phosphorylating agents, e.g., (PhO)₂P(O)Cl, were achieved at positions 3', 5', and N-6 using appropriate starting materials for unambiguous synthesis. There is a difference in the reactivity of the different functions in these mols. with a preference of the 5'-OH followed by 6-NH₂ and then 3'-OH in the 3rd place. UV and CD spectral data and pK_a values of various adenosine and 2'-deoxyadenosine phosphotriesters prep'd. are given.

L5 ANSWER 116 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 78098-57-4 REGISTRY
CN 3'-Adenylic acid, 2'-deoxy-N-(diphenoxyphosphinyl)-5'-O-[(4-methoxyphenyl)diphenylmethyl]-, diphenyl ester (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C54 H47 N5 O10 P2
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 95:25488 Nucleotides. XIII. Phosphorylations of adenosine and 2'-deoxyadenosine by phosphorochloridates. Charubala, Ramamurthy; Pfleiderer, Wolfgang (Fak. Chem., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger.). Heterocycles, 15(2), 761-76 (English) 1981. CODEN: HTCYAM. ISSN: 0385-5414.

AB Phosphorylations of adenosine and 2'-deoxyadenosine by various phosphorylating agents, e.g., (PhO)2P(O)Cl, were achieved at positions 3',5', and N-6 using appropriate starting materials for unambiguous synthesis. There is a difference in the reactivity of the different functions in these mols. with a preference of the 5'-OH followed by 6-NH2 and then 3'-OH in the 3rd place. UV and CD spectral data and pKa values of various adenosine and 2'-deoxyadenosine phosphotriesters prep'd. are given.

L5 ANSWER 117 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 78098-56-3 REGISTRY

CN 3'-Adenylic acid, 2'-deoxy-N-(diphenoxyphosphinyl)-, diphenyl ester, 5'-(diphenyl phosphate) (9CI) (CA INDEX NAME)

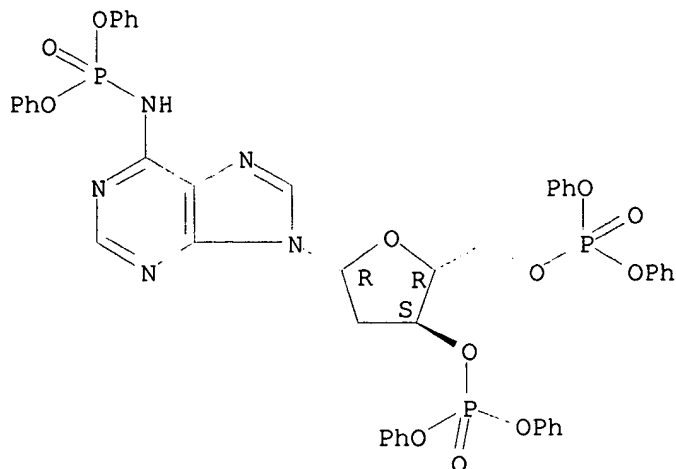
FS STEREOSEARCH

MF C46 H40 N5 O12 P3

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

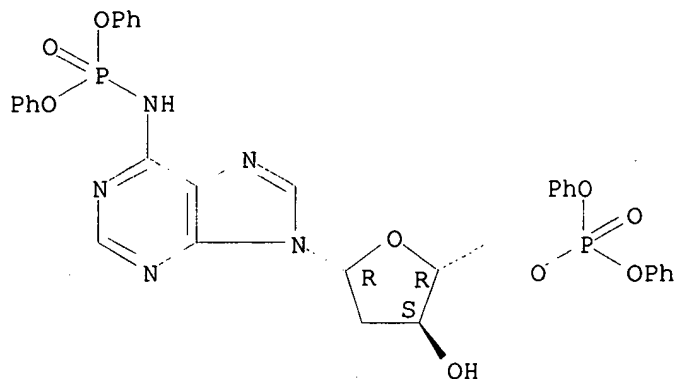
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 95:25488 Nucleotides. XIII. Phosphorylations of adenosine and 2'-deoxyadenosine by phosphorochloridates. Charubala, Ramamurthy; Pfleiderer, Wolfgang (Fak. Chem., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger.). Heterocycles, 15(2), 761-76 (English) 1981. CODEN: HTCYAM. ISSN: 0385-5414.

AB Phosphorylations of adenosine and 2'-deoxyadenosine by various phosphorylating agents, e.g., (PhO)₂P(O)Cl, were achieved at positions 3', 5', and N-6 using appropriate starting materials for unambiguous synthesis. There is a difference in the reactivity of the different functions in these mols. with a preference of the 5'-OH followed by 6-NH₂ and then 3'-OH in the 3rd place. UV and CD spectral data and pK_a values of various adenosine and 2'-deoxyadenosine phosphotriesters prep'd. are given.

L5 ANSWER 118 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 78098-55-2 REGISTRY
CN 5'-Adenylic acid, 2'-deoxy-N-(diphenoxyposphinyl)-, diphenyl ester (9CI)
(CA INDEX NAME)
FS STEREOSEARCH
MF C34 H31 N5 O9 P2
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

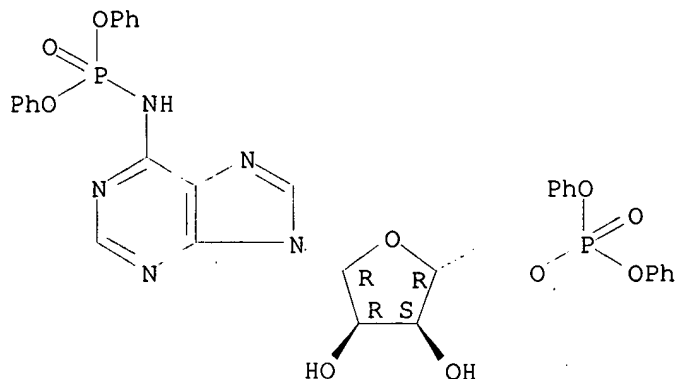
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 95:25488 Nucleotides. XIII. Phosphorylations of adenosine and 2'-deoxyadenosine by phosphorochloridates. Charubala, Ramamurthy; Pfeleiderer, Wolfgang (Fak. Chem., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger.). Heterocycles, 15(2), 761-76 (English) 1981. CODEN: HTCYAM. ISSN: 0385-5414.

AB Phosphorylations of adenosine and 2'-deoxyadenosine by various phosphorylating agents, e.g., (PhO)2P(O)Cl, were achieved at positions 3', 5', and N-6 using appropriate starting materials for unambiguous synthesis. There is a difference in the reactivity of the different functions in these mols. with a preference of the 5'-OH followed by 6-NH2 and then 3'-OH in the 3rd place. UV and CD spectral data and pKa values of various adenosine and 2'-deoxyadenosine phosphotriesters prep'd. are given.

L5 ANSWER 119 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 78098-53-0 REGISTRY
CN 5'-Adenylic acid, N-(diphenoxyphosphinyl)-, diphenyl ester (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C34 H31 N5 O10 P2
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.



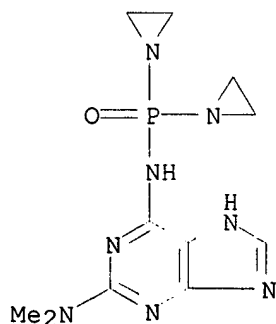
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 95:25488 Nucleotides. XIII. Phosphorylations of adenosine and 2'-deoxyadenosine by phosphorochloridates. Charubala, Ramamurthy; Pfleiderer, Wolfgang (Fak. Chem., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger.). Heterocycles, 15(2), 761-76 (English) 1981. CODEN: HTCYAM. ISSN: 0385-5414.

AB Phosphorylations of adenosine and 2'-deoxyadenosine by various phosphorylating agents, e.g., (PhO)₂P(O)Cl, were achieved at positions 3', 5', and N-6 using appropriate starting materials for unambiguous synthesis. There is a difference in the reactivity of the different functions in these mols. with a preference of the 5'-OH followed by 6-NH₂ and then 3'-OH in the 3rd place. UV and CD spectral data and pK_a values of various adenosine and 2'-deoxyadenosine phosphotriesters prepd. are given.

L5 ANSWER 120 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 77931-46-5 REGISTRY
CN Phosphinic amide, P,P-bis(1-aziridinyl)-N-[2-(dimethylamino)-1H-purin-6-yl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C11 H17 N8 O P
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER
(*File contains numerically searchable property data)



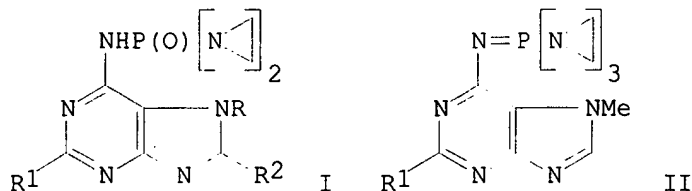
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 95:7223 Synthesis and antineoplastic activity of 6-diethylenimidophosphamido- and 6-triethyleniminophosphazopurines. Glushkov, R. G.; Nikolaeva, L. A.; Golovchinskaya, E. S.; Chernov, V. A.; Kravchenko, A. I.; Kozlova, O. V.; Gutorov, L. A. (Vses. Nauchno-Issled. Khim.-Farm. Inst., Moscow, USSR). Khim.-Farm. Zh., 15(3), 16-20 (Russian) 1981. CODEN: KHFZAN. ISSN: 0023-1134.

GI



AB The title compds. I (R = Me, PhCH₂, H, R₁ = NMe₂, pyrrolidino, 2,2-dimethylpyrrolidino, piperidino, morpholino, R₂ = H, Cl, morpholino) and II (R₁ = NMe₂, pyrrolidino, 2,2-dimethylpyrrolidino) were obtained in 47.1-81.0% yields (I) and 48.7-61.3% yields (II) by phosphorylation of the amino group of a 6-aminopurine by POCl₃-aziridine and PCl₅-aziridine, resp. I and II were effective neoplasm inhibitors for Sarcoma 45 and Sarcoma 180 in white mice and rats.

L5 ANSWER 121 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 74242-14-1 REGISTRY

CN 2-Propenamide, N-[2-[6-[(diphenylphosphinothioyl)amino]-9H-purin-9-yl]ethyl]-, homopolymer (9CI) (CA INDEX NAME)

MF (C22 H21 N6 O P S)x

CI PMS

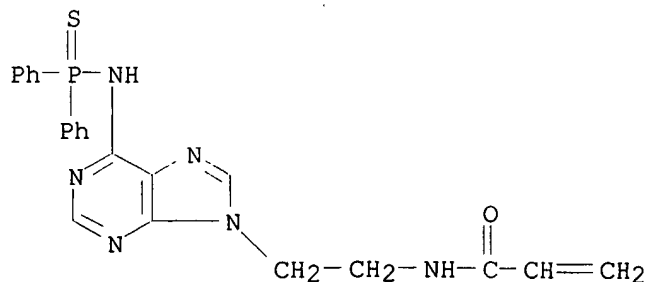
PCT Polyacrylic

LC STN Files: CA, CAPLUS

CM 1

CRN 74242-13-0

CMF C22 H21 N6 O P S



1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

Searched by: Mary Hale 308-4258 CM-1 1E01

REFERENCE 1: 93:72346 Functional monomers and polymers. 77. Synthesis and polymerization of acryloylamino derivatives of nucleic acid bases. Kondo, Koichi; Tanioku, Shozo; Takemoto, Kiichi (Fac. Eng., Osaka Univ., Suita, Japan). Makromol. Chem., Rapid Commun., 1(5), 303-6 (English) 1980. CODEN: MCRCD4.

AB Purinylethylacrylamide derivs. and N-[4-(4-ethoxy-2-oxo-1,2-dihydropyrimidin-1-ylmethyl)phenyl]acrylamide [74242-05-0] (prepd. from acrylic anhydride and the appropriate amine) were subjected to H-transfer polymn. for 20 h at 100.degree. in DMF, DMSO, or pyridine, giving products with mol. wt. 2000 (MeOH-sol.) and 8000 (MeOH-insol.).

L5 ANSWER 122 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 74242-13-0 REGISTRY

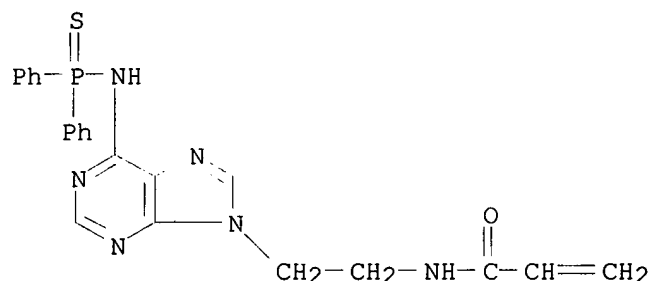
CN 2-Propenamide, N-[2-[6-[(diphenylphosphinothioyl)amino]-9H-purin-9-yl]ethyl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C22 H21 N6 O P S

CI COM

LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 93:72346 Functional monomers and polymers. 77. Synthesis and polymerization of acryloylamino derivatives of nucleic acid bases. Kondo, Koichi; Tanioku, Shozo; Takemoto, Kiichi (Fac. Eng., Osaka Univ., Suita, Japan). Makromol. Chem., Rapid Commun., 1(5), 303-6 (English) 1980. CODEN: MCRCD4.

AB Purinylethylacrylamide derivs. and N-[4-(4-ethoxy-2-oxo-1,2-dihydropyrimidin-1-ylmethyl)phenyl]acrylamide [74242-05-0] (prepd. from acrylic anhydride and the appropriate amine) were subjected to H-transfer polymn. for 20 h at 100.degree. in DMF, DMSO, or pyridine, giving products with mol. wt. 2000 (MeOH-sol.) and 8000 (MeOH-insol.).

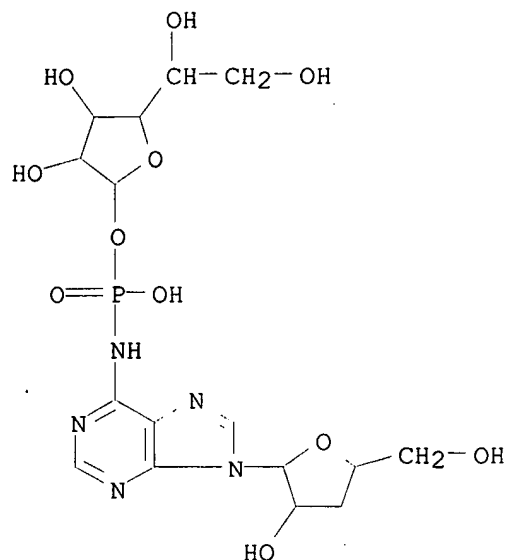
L5 ANSWER 123 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 72666-23-0 REGISTRY

CN D-Glucofuranose, 1-[hydrogen [9-(3-deoxy-.beta.-D-threo-pentofuranosyl)-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

MF C16 H24 N5 O11 P

LC STN Files: CA, CAPLUS, TOXCENTER



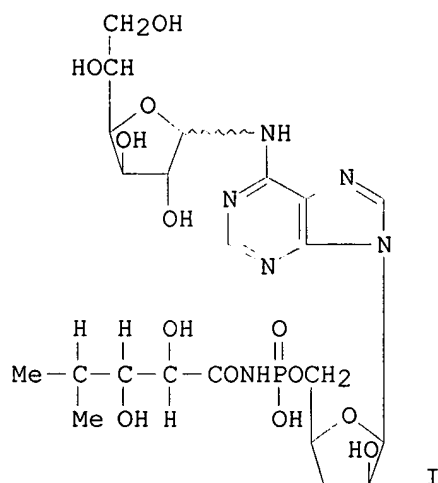
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)

2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 95:36238 Substituents at N6 and C-5' control selective uptake and toxicity of the adenine-nucleotide bacteriocin, agrocin 84, in agrobacteria. Murphy, Peter J.; Tate, Max E.; Kerr, Allen (Waite Agric. Res. Inst., Univ. Adelaide, Adelaide, 5064, Australia). Eur. J. Biochem., 115(3), 539-43 (English) 1981. CODEN: EJBCAI. ISSN: 0014-2956.

GI



I

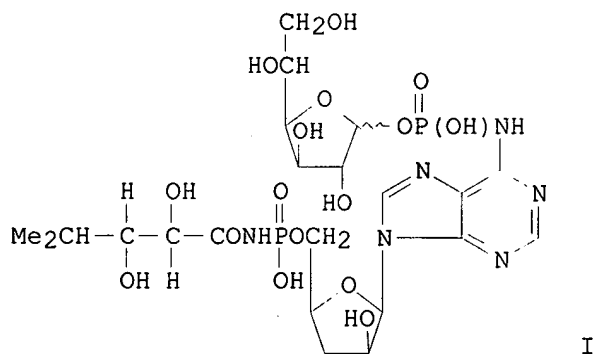
AB The inhibition of a sensitive strain of Agrobacterium radiobacter by the nucleotide bacteriocin agrocin 84 (I) [59111-78-3] was detd., and a structure-function study of the I mol. was undertaken. Two I nucleotide fragments lacking either the N6 [77822-25-4] or 5'-phosphoramidate [72666-23-0] substituents were used in uptake studies of [32P2]I,

Searched by: Mary Hale 308-4258 CM-1 1E01

establishing that the plasmid-controlled, strain-specific uptake of I is detd. by the N6-D-glucofuranosyloxyphosphoramidate substituent. This was further supported by the markedly reduced uptake of the ^{32}P -labeled fragment lacking the N6-substituent. Equil. dialysis studies indicated that the N6-substituent is recognized by a binding protein involved in the uptake of I into sensitive strains. The nucleotide fragment bearing the N6-substituent was a competitive inhibitor for the uptake of I in vivo with a $K_i = 1.0 \times 10^{-7}\text{M}$ and was itself selectively transported into a sensitive strain at a rate comparable with I; unlike I however, it is nontoxic. By contrast, the fragment bearing the 5'-phosphoramidate was taken up by both sensitive and insensitive strains at a barely measurable rate and was toxic to both.

REFERENCE 2: 92:89158 Adenine N6-substituent of agrocin 84 determines its bacteriocin-like specificity. Tate, M. E.; Murphy, P. J.; Roberts, W. P.; Kerr, A. (Waite Agric. Res. Inst., Univ. Adelaide, Glen Osmond, 5064, Australia). Nature (London), 280(5724), 697-9 (English) 1979. CODEN: NATUAS. ISSN: 0028-0836.

GI



AB For the pathogenic strain 57A of *Agrobacterium*, agrocin 84 (I) [59111-78-3] was 360 times more potent than its nucleotide fragment, nucleoside 5'-phosphoramidate (II) [72666-24-1]. The nonpathogenic strain 57 was not inhibited by agrocin 84 at molarities at which II readily gave inhibition (3.2×10^8 agrocin units/mol). These data show that a 5'-phosphoryl link from the fraudulent nucleoside core 9-(3'-deoxy- β -D-threo-pentofuranosyl)adenine to the amide group of D-threo-2,3-dihydroxy-4-methylpentanamide was required for antibiotic activity, but bacteriocin-like specificity was conferred by a D-glucofuranosyloxyphosphoryl substituent at N6 of adenine.

L5 ANSWER 124 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 66723-17-9 REGISTRY

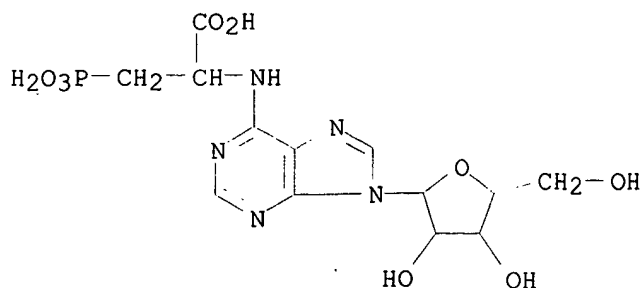
CN Alanine, 3-phosphono-N-(9- β -D-ribofuranosyl-9H-purin-6-yl)- (9CI)
(CA INDEX NAME)

OTHER CA INDEX NAMES:

CN DL-Alanine, 3-phosphono-N-(9- β -D-ribofuranosyl-9H-purin-6-yl)-

MF C13 H18 N5 O9 P

LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

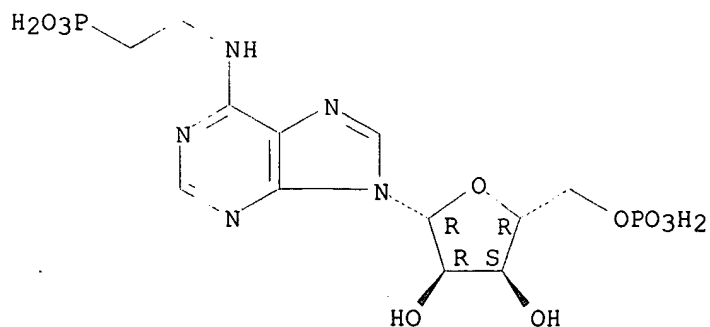
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 89:38622 Inhibition of adenylosuccinase by adenylophosphonopropionate and related compounds. Brand, Larry M.; Lowenstein, John M. (Grad. Dep. Biochem., Brandeis Univ., Waltham, Mass., USA). Biochemistry, 17(8), 1365-70 (English) 1978. CODEN: BICHAW. ISSN: 0006-2960.

AB Adenylosuccinase from muscle, liver, and yeast was strongly inhibited by the substrate analog, adenylophosphonopropionate [N6-(DL-1-carboxy-2-phosphonoethyl)AMP]. The inhibition was freely reversible and of the competitive type, with apparent K_i values of 5.4-86 nM depending on the source of enzyme. Ratios of K_m/K_i with adenylosuccinate as substrate fell in the range 44-1350. Comparison of 4 carboxyl analogs of adenylosuccinate with the corresponding phosphonate analogs showed that the phosphonates were much better inhibitors. Adenylosuccinate analogs in which the β -carboxyl was replaced by other functional groups were much poorer inhibitors. The exceptionally high affinity of adenylosuccinase for adenylophosphonopropionate appears to involve the dianion of the phosphonate group.

L5 ANSWER 125 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 66723-16-8 REGISTRY
CN 5'-Adenylic acid, N-(2-phosphonoethyl)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C12 H19 N5 O10 P2
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.



Searched by: Mary Hale 308-4258 CM-1 1E01

****PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT****

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 89:38622 Inhibition of adenylosuccinase by adenylophosphonopropionate and related compounds. Brand, Larry M.; Lowenstein, John M. (Grad. Dep. Biochem., Brandeis Univ., Waltham, Mass., USA). Biochemistry, 17(8), 1365-70 (English) 1978. CODEN: BICHAW. ISSN: 0006-2960.

AB Adenylosuccinase from muscle, liver, and yeast was strongly inhibited by the substrate analog, adenylophosphonopropionate [N6-(DL-1-carboxy-2-phosphonoethyl)AMP]. The inhibition was freely reversible and of the competitive type, with apparent K_i values of 5.4-86 nM depending on the source of enzyme. Ratios of K_m/K_i with adenylosuccinate as substrate fell in the range 44-1350. Comparison of 4 carboxyl analogs of adenylosuccinate with the corresponding phosphonate analogs showed that the phosphonates were much better inhibitors. Adenylosuccinate analogs in which the β -carboxyl was replaced by other functional groups were much poorer inhibitors. The exceptionally high affinity of adenylosuccinase for adenylophosphonopropionate appears to involve the dianion of the phosphonate group.

L5 ANSWER 126 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 66723-15-7 REGISTRY

CN Butanoic acid, 4-phosphono-2-[[9-(5-O-phosphono- β -D-ribofuranosyl)-9H-purin-6-yl]amino]- (9CI) (CA INDEX NAME)

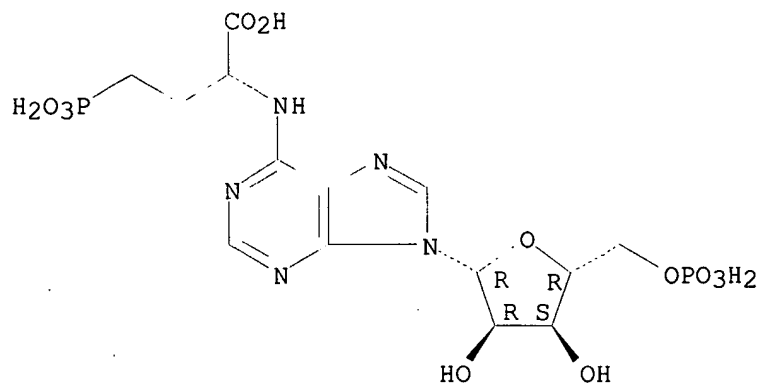
FS STEREOSEARCH

MF C14 H21 N5 O12 P2

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

Absolute stereochemistry.



****PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT****

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

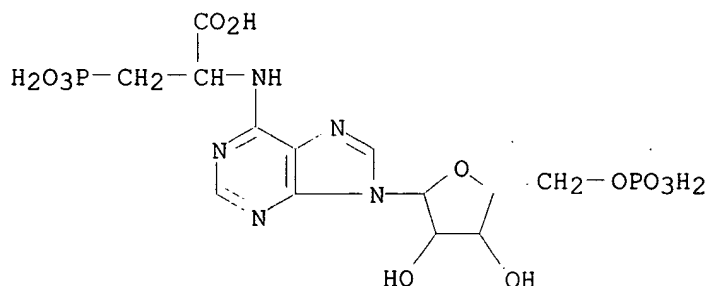
REFERENCE 1: 89:38622 Inhibition of adenylosuccinase by adenylophosphonopropionate and related compounds. Brand, Larry M.; Lowenstein, John M. (Grad. Dep. Biochem., Brandeis Univ., Waltham, Mass., USA). Biochemistry, 17(8), 1365-70 (English) 1978. CODEN: BICHAW. ISSN: 0006-2960.

AB Adenylosuccinase from muscle, liver, and yeast was strongly inhibited by

Searched by: Mary Hale 308-4258 CM-1 1E01

the substrate analog, adenylophosphonopropionate [N6-(DL-1-carboxy-2-phosphonoethyl)AMP]. The inhibition was freely reversible and of the competitive type, with apparent K_i values of 5.4-86 nM depending on the source of enzyme. Ratios of K_m/K_i with adenylosuccinate as substrate fell in the range 44-1350. Comparison of 4 carboxyl analogs of adenylosuccinate with the corresponding phosphonate analogs showed that the phosphonates were much better inhibitors. Adenylosuccinate analogs in which the .beta.-carboxyl was replaced by other functional groups were much poorer inhibitors. The exceptionally high affinity of adenylosuccinase for adenylophosphonopropionate appears to involve the dianion of the phosphonate group.

L5 ANSWER 127 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 66723-09-9 REGISTRY
 CN Alanine, 3-phosphono-N-[9-(5-O-phosphono-.beta.-D-ribofuranosyl)-9H-purin-6-yl]- (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN DL-Alanine, 3-phosphono-N-[9-(5-O-phosphono-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-
 MF C13 H19 N5 O12 P2
 LC STN Files: BEILSTEIN*, CA, CAPLUS
 (*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

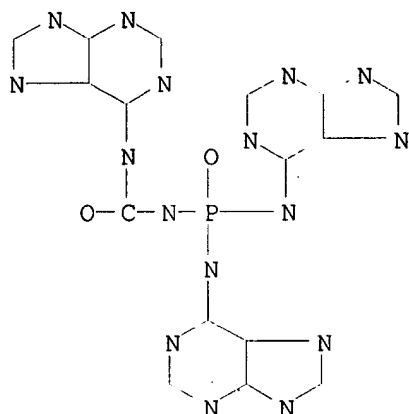
REFERENCE 1: 89:38622 Inhibition of adenylosuccinase by adenylophosphonopropionate and related compounds. Brand, Larry M.; Lowenstein, John M. (Grad. Dep. Biochem., Brandeis Univ., Waltham, Mass., USA). Biochemistry, 17(8), 1365-70 (English) 1978. CODEN: BICHAW. ISSN: 0006-2960.

AB Adenylosuccinase from muscle, liver, and yeast was strongly inhibited by the substrate analog, adenylophosphonopropionate [N6-(DL-1-carboxy-2-phosphonoethyl)AMP]. The inhibition was freely reversible and of the competitive type, with apparent K_i values of 5.4-86 nM depending on the source of enzyme. Ratios of K_m/K_i with adenylosuccinate as substrate fell in the range 44-1350. Comparison of 4 carboxyl analogs of adenylosuccinate with the corresponding phosphonate analogs showed that the phosphonates were much better inhibitors. Adenylosuccinate analogs in which the .beta.-carboxyl was replaced by other functional groups were much poorer inhibitors. The exceptionally high affinity of adenylosuccinase for adenylophosphonopropionate appears to involve the dianion of the phosphonate group.

L5 ANSWER 128 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 64196-71-0 REGISTRY

Searched by: Mary Hale 308-4258 CM-1 1E01

CN Urea, N-[bis(1H-purin-6-ylamino)phosphinyl]-N'-1H-purin-6-yl- (9CI) (CA
INDEX NAME)
MF C16 H13 N16 O2 P
LC STN Files: CA, CAPLUS



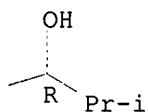
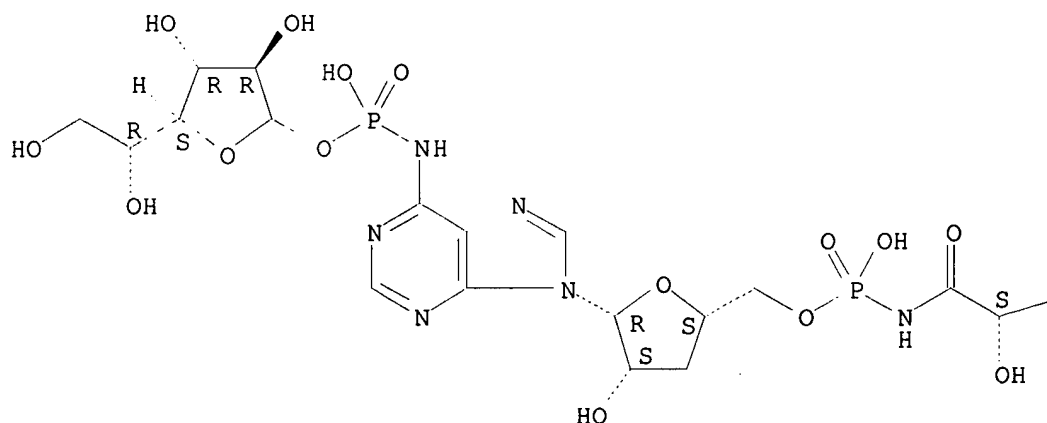
*** FRAGMENT DIAGRAM IS INCOMPLETE ***

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 87:201587 N-Purinyl-N'-[bis(purinylamino)phosphonyl]ureas.
Gubnitskaya, E. S.; Cherkasov, V. M.; Kurilenko, L. K.; Loseva, I. M.;
Derkach, G. I. (Institute of Organic Chemistry, Academy of Sciences,
Ukrainian S.S.R., USSR). U.S.S.R. SU 412765 19770705 (Russian). CODEN:
URXXAF. APPLICATION: SU 1970-1457304 19700709.
AB The title compds. were prepd. by treatment of Cl₂P(O)NCO with substituted
6-aminopurines in the presence of Et₃N.

L5 ANSWER 129 OF 140 REGISTRY COPYRIGHT 2002 ACS
RN 59111-78-3 REGISTRY
CN D-Glucofuranose, 1-[hydrogen [9-[3-deoxy-5-O-[[[(4,5-dideoxy-4-methyl-D-
threo-pentonoyl)amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-
purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Agrocin 84
OTHER NAMES:
CN Mono-D-glucofuranosyl [9-[3-deoxy-5-O-[[[(4,5-dideoxy-4-methyl-D-threo-
pentonoyl)amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-purin-
6-yl]phosphoramidate
FS STEREOSEARCH
MF C22 H36 N6 O16 P2
LC STN Files: AGRICOLA, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT,
CAPLUS, EMBASE, MEDLINE, TOXCENTER

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

43 REFERENCES IN FILE CA (1967 TO DATE)
43 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 136:184004 Total synthesis of agrocin 84 and phosmidosine as naturally occurring nucleotidic antibiotics having P-N bond linkages. Sekine, Mitsuo; Moriguchi, Tomohisa; Wada, Takeshi; Seio, Kohji (Department of Life Science, Tokyo Institute of Technology, Yokohama, 226-8501, Japan). Yuki Gosei Kagaku Kyokaishi, 59(11), 1109-1120 (English) 2001. CODEN: YGKKAE. ISSN: 0037-9980. Publisher: Yuki Gosei Kagaku Kyokai.

AB A review with refs. This review deals with our recent studies of the synthesis of naturally occurring nucleic acid derivs. having P-N linkages. The total synthesis of a nucleotidic antibiotic, agrocin 84, having two different types of unique phosphoramidate bonds is described in detail. Phosmidosine is an antibiotic that has an antifungal activity and has a rare O-methylated phosphoramidate structure. Dinitrophenyl This compd. was also successfully synthesized by use of 5-(3,5-dinitrophenyl)-1H-tetrazole (DNPT) as the powerful activator of an N-prolyl phosphorodiamidite deriv. that was condensed with an 8-oxoadenosine deriv. Several related compds. were also synthesized. These phosmidosine derivs. were found to exhibit significant antitumor activities. In connection with these studies, the synthesis and biol. properties of aminoacylamido-AMP derivs. having N-P

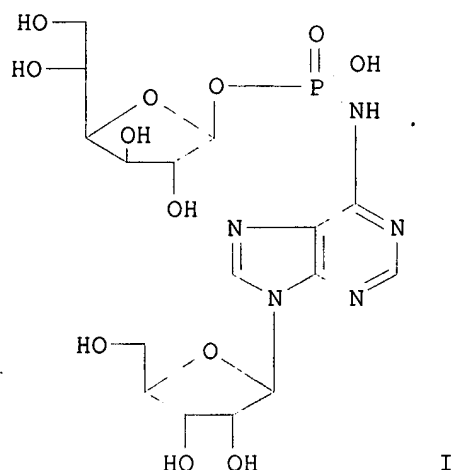
bonds as stable analogs of aminoacyl-AMP are also described.

- REFERENCE 2: 132:279438 Synthesis of nucleotide antibiotics having N-acyl phosphoramidate linkages. Moriguchi, Tomohisa; Asai, Norio; Wada, Takeshi; Sekine, Mitsuo (Department of Life Science, Tokyo Institute of Technology, Yokohama, 226-8501, Japan). Nucleic Acids Symposium Series, 42 (Twenty-sixth Symposium on Nucleic Acids Chemistry, 1999), 15-16 (English) 1999. CODEN: NACSD8. ISSN: 0261-3166. Publisher: Oxford University Press.
- AB A symposium on the synthesis of nucleotide antibiotics having N-acyl phosphoramidate linkages. The key reaction, the construction of the N-acyl phosphoramidate linkage was achieved by the reaction of nucleoside 5'-phosphoramidite derivs. with carboxamide derivs. in the presence of 5-(3,5-dinitrophenyl)-1H-tetrazole as a very effective activator. By use of this activator, phosmidosine was synthesized by condensation of an appropriately protected 8-oxoadenosine 5'-O-phosphoramidite deriv. with an N-protected prolinamide deriv. In the case of agrocin 84, the two P-N bonds were constructed progressively. The N-acyl phosphoramidate linkage at the 5'-position of the ribose moiety was similarly synthesized. After phosphorylation of the amino group of the adenine moiety, a fully protected agrocin 84 deriv., which would be converted to agrocin 84, was successfully synthesized.
- REFERENCE 3: 129:184979 Diversity of plasmids of *Agrobacterium tumefaciens* isolated from fruit trees in Poland. Pulawska, J.; Malinowski, T.; Sobiczewski, P. (Research Institute Pomology Floriculture, Skierniewice, 96100, Pol.). Journal of Phytopathology, 146(8-9), 465-468 (English) 1998. CODEN: JPHYEB. ISSN: 0931-1785. Publisher: Blackwell Wissenschafts-Verlag GmbH.
- AB Plasmid DNA was isolated from 11 strains of *Agrobacterium tumefaciens* originated from 6 fruit tree species of various locations in Poland. 1 - 4 Plasmids were consistently isolated from all studied strains. Plasmid sizes varied from about 27 to about 315 kbp. Some of the strains possessed similar plasmid profiles. The lack of any clear relationship between plasmid profiles of strains and their virulence, sensitivity to agrocin 84, biovar and origin was obsd.
- REFERENCE 4: 128:98395 Characterization of the *acc* operon from the nopaline-type Ti plasmid pTiC58, which encodes utilization of agrocinopines A and B and susceptibility to agrocin 84. Kim, Heenam; Farrand, Stephen K. (Department of Microbiology, University of Illinois at Urbana-Champaign, Urbana, IL, 61801, USA). Journal of Bacteriology, 179(23), 7559-7572 (English) 1997. CODEN: JOBAAY. ISSN: 0021-9193. Publisher: American Society for Microbiology.
- AB The *acc* locus from the Ti plasmid pTiC58 confers utilization of and chemotaxis toward agrocinopines A and B (A+B), as well as susceptibility to a highly specific antiagrobacterial antibiotic, agrocin 84. DNA sequence analyses revealed that *acc* is composed of eight open reading frames, *accR* and *accA* through *accG*. Previous work showed that *accR* encodes the repressor which regulates this locus, and *accA* codes for the periplasmic binding protein of the agrocinopine transport system (S. Beck Von Bodman, G. T. Hayman, and S. K. Farrand, Proc. Natl. Acad. Sci. USA 89:643-647, 1992; G. T. Hayman, S. Beck Von Bodman, H. Kim, P. Jiang, and S. K. Farrand, J. Bacteriol. 175:5575-5584, 1993). The predicted proteins from *accA* through *accE*, as a group, have homol. to proteins that belong to the ABC-type transport system superfamily. The predicted product of *accF* is related to UgpQ of *Escherichia coli*, which is a glycerophosphoryl diester phosphodiesterase, and also to agrocinopine synthase coded for by *acs* located on the T-DNA. The translated product of *accG* is related to myo-inositol 1 (or 4) monophosphatases from various eukaryotes. Analyses of insertion mutations showed that *accA* through *accE* are required for transport of both agrocin 84 and agrocinopines A+B, while *accF* and *accG*

are required for utilization of the opines as the sole source of carbon. Mutations in accF or accG did not abolish transport of agrocin 84, although we obsd. slower removal of the antibiotic from the medium by the accF mutant compared to the wild type. However, the insertion mutation in accF abolished detectable uptake of agrocinopines A+B. A mutation in accG had no effect on transport of the opines. The accF mutant was not susceptible to agrocin 84 although it took up the antibiotic. This finding suggests that agrocin 84 is activated by AccF after being transported into the bacterial cell.

REFERENCE 5: 126:47468 New Nucleoside-Sugar Conjugates: 6-N-Glycosyloxyphosphorylated Adenosine Derivatives as Partial Structures of Agrocin 84. Moriguchi, Tomohisa; Wada, Takeshi; Sekine, Mitsuo (Department of Life Science, Tokyo Institute of Technology, Yokohama, 226, Japan). Journal of Organic Chemistry, 61(26), 9223-9228 (English) 1996. CODEN: JOCEAH. ISSN: 0022-3263. Publisher: American Chemical Society.

GI



AB We report the first successful prepn. of glucofuranosyloxyphosphoryl adenosine I as a partial structure of agrocin 84 via a two-step phosphorylation of 2',3',5'-tri-O-benzoyl adenosine with a 2,3,5,6-tetra-O-acetylglucofuranoside 1-O-phosphoramidite deriv. that has a 2-(trimethylsilyl)ethyl group as the phosphate protecting group. The stabilities of these 6-N-[(glycos-1-yloxy)phosphoryl]adenosine derivs. under acidic, basic, and thermal conditions are described. In particular, we found that the O-P bond of these sugar-nucleoside conjugates was selectively cleaved by treatment with 0.1 M NaOH to give 6-N-phosphoryl adenosine, while acidic treatment gave directly adenosine with cleavage of the P-N bond.

REFERENCE 6: 125:2931 Spontaneous transfer of the Ti plasmid of Agrobacterium tumefaciens and the nopaline catabolism plasmid of A. radiobacter strain K84 in crown gall tissue. Vicedo, Begonya; Lopez, Maria Jose; Asins, Maria Jose; Lopez, Maria M. (Instituto Valenciano de Investigaciones Agrarias, Moncada, 46113, Spain). Phytopathology, 86(5), 528-534 (English) 1996. CODEN: PHYTAJ. ISSN: 0031-949X.

AB Spontaneous transfer of the Ti plasmid from Agrobacterium tumefaciens to strain K84 of A. radiobacter was obsd. and studied for the first time in an expt. on biol. control of crown gall. This transfer was detected in a tumor from a K84-treated plant grown in soil inoculated with a nopaline strain of A. tumefaciens biovar 1 sensitive to agrocin 84. The

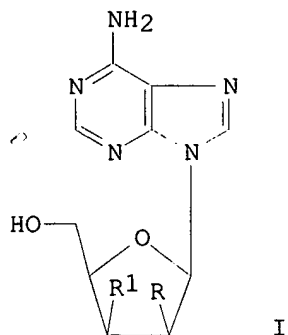
transconjugant strain was virulent and produced agrocin 84. Southern blot hybridization anal. with several probes (T-DNA and right adjacent regions and vir genes) showed important changes at the Ti plasmid, suggesting that recombination between Ti plasmid and pAtK84b in K84 could have happened, resulting in a new Ti plasmid. Transfer of both plasmids of strain K84, pAtK84b and pAgK84, responsible for nopaline catabolism and agrocin 84 prodn., resp., to *A. tumefaciens* also was detected in isolates from the same tumor. Southern blot hybridization of plasmids from one of these avirulent isolates with a nopaline plasmid-specific probe of strain K84 indicated there was a replacement of Ti plasmid by pAtK84b in *A. tumefaciens*, explaining its avirulence. These results show that plasmid exchanges can occur spontaneously between *A. tumefaciens* and *A. radiobacter*. This kind of transfer generates genetic diversity in *Agrobacterium* and may influence the biocontrol efficiency of *A. radiobacter*.

REFERENCE 7: 122:98736 Organization and expression of the genes on pAgK84 that encode production of agrocin 84. Wang, Chang-Lin; Farrand, Stephen K.; Hwang, Ingyu (Department of Plant Pathology, University of Illinois, Urbana, 61801, USA). *Mol. Plant-Microbe Interact.*, 7(4), 472-81 (English) 1994. CODEN: MPMIEL. ISSN: 0894-0282.

AB Agrocin 84 biosynthesis genes located in a 21-kb segment of pAgK84 were characterized by mutagenesis with Tn3HoHo1 and complementation anal. Three overlapping fragments of the 21-kb segment, cloned into pRK415 or pLAFR6, were mutagenized with Tn3HoHo1, and 94 independent insertions were mapped and oriented. A series of merodiploid strains, each contg. a Tn5 insertion in pAgK84 affecting agrocin 84 biosynthesis, and a clone contg. a Tn3HoHo1 insertion that blocks antibiotic prodn. in homogenotes were constructed to det. the no. of complementation groups involved in agrocin 84 biosynthesis. Five complementation groups were identified and named agnA through agnE. Anal. of lacZ fusions formed by the Tn3HoHo1 inserts indicated that all of the loci except agnD are transcribed in an anticlockwise direction. Insertions carried on clones and insertions marker-exchanged into pAgK84 had similar patterns of expression. The five agn loci were not expressed at significant levels in *Escherichia coli* DH5.alpha. grown in minimal or rich media. Levels of expression in *Agrobacterium tumefaciens* NT1 differed for each region; agnA was expressed at relatively high levels, agnC and agnE at intermediate levels, and agnB and agnD at very low levels. Similar patterns of expression were obsd. in minimal media, regardless of the carbon source, and at neutral and acidic pHs. Expression levels were lower in cells grown in rich medium. The level of expression of each agn locus was not affected by the presence of other agn genes or by the presence or absence of the large nopaline plasmid pAtK84b, present in strain K84. Nor were the levels of expression influenced by the addn. of opines or root exudates to the culture media. All five agn loci were expressed at all growth stages, and expression reached max. levels during late exponential growth. The agn loci were expressed in planta, and the patterns of expression were similar to those seen in bacteria grown in vitro. The presence of pAtK84b did not affect agn expression in planta.

REFERENCE 8: 120:271041 Nucleic acid related compounds. 81. Syntheses of 9-(3-deoxy-.beta.-D-threo-pentofuranosyl)adenine, the core nucleoside of the extraordinarily selective antibiotic agrocin 84, and simplified structural component analogs. Vinayak, Ravi; Hansske, Fritz; Robins, Morris J. (Dep. Chem., Univ. Alberta, Edmonton, AB, Can.). *J. Heterocycl. Chem.*, 30(5), 1181-9 (English) 1993. CODEN: JHTCAD. ISSN: 0022-152X.

GI



AB Alternative syntheses of (deoxy-.beta.-D-threo-pentofuranosyl)adenine I (R = OH, R1 = H) (II), the core nucleoside of agrocin 84 and its 2'-deoxy threo isomer I (R = H, R1 = OH) (III) were devised: (1) direct conversion of 9-(.beta.-D-arabinofuranosyl)adenine into 9-(2,3-anhydro-.beta.-D-lyxofuranosyl)adenine and regioselective opening of its oxirane ring with sodium borohydride to give II and III (.apprx.7.5:1); (2) treatment of adenosine with sodium hydride and 2,4,6-triisopropylbenzenesulfonyl chloride, and subjection of the resulting 2'(3')-sulfonates to the reductive [1,2]-hydride shift rearrangement with lithium triethylborohydride to give II and III (.apprx.2:1); and (3) subjection of the phenoxythiocarbonyl esters of 9-[2(3),5-bis-O-(tert-butyl)dimethylsilyl]-.beta.-D-arabinofuranosyl]adenine to Barton deoxygenation, and deprotection to give II and 2'-deoxyadenosine (.apprx.5:1). Methods (2) and (3) gave lower yields. Syntheses of simplified 6-N- and 5'-O-adenosine phosphoramidate model compds. were explored to examine potential access to such features in the structure proposed for agrocin 84.

REFERENCE 9: 120:24582 Genetic analysis of the agrocinopine catabolic region of *Agrobacterium tumefaciens* Ti plasmid pTiC58, which encodes genes required for opine and agrocin 84 transport. Hayman, G. Thomas; Beck von Bodman, Susanne; Kim, Heenam; Jiang, Ping; Farrand, Stephen K. (Med. Cent., Loyola Univ., Maywood, IL, 60153, USA). *J. Bacteriol.*, 175(17), 5575-84 (English) 1993. CODEN: JOBAAY. ISSN: 0021-9193.

AB The acc region, subcloned from pTiC58 of classical nopaline and agrocinopine A and B *Agrobacterium tumefaciens* C58, allowed agrobacteria to grow using agrocinopine B as the sole source of carbon and energy. Acc is .apprx.6 kb in size. It consists of .gtoreq.5 genes, accA through accE, as defined by complementation anal. using subcloned fragments and transposon insertion mutations of acc carried on different plasmids within the same cells. All 5 regions are required for agrocin 84 sensitivity, and .gtoreq.4 are required for agrocinopine and agrocin 84 uptake. The complementation results are consistent with the hypothesis that each of the 5 regions is sep. transcribed. Maxicell expts. showed that the first of these genes, accA, encodes a 60-kDa protein. Anal. of osmotic shock fractions showed this protein to be located in the periplasm. The DNA sequence of the accA region revealed an open reading frame encoding a predicted polypeptide of 59,147 Da. The amino acid sequence encoded by this open reading frame is similar to the periplasmic binding proteins OppA and DppA of *Escherichia coli* and *Salmonella typhimurium* and OppA of *Bacillus subtilis*.

REFERENCE 10: 120:24551 Functional and mutated agrocinopine synthase genes on octopine T-DNAs. Paulus, Francois; Otten, Leon (Plant Mol. Biol. Lab., CNRS, Strasbourg, 67084, Fr.). *Mol. Plant-Microbe Interact.*, 6(3), 393-402 (English) 1993. CODEN: MPMIEL. ISSN: 0894-0282.

AB Agrocinnopine synthase genes have so far been detected only on the *Agrobacterium tumefaciens* nopaline Ti plasmid pTiC58 and on the *A. rhizogenes* Ri plasmid pRiA4. The TA region of the octopine/cucumopine (o/c) *A. vitis* Ti plasmid pTiTm4 strongly resembles the TL DNA of biotype I octopine Ti plasmids. In addn., it carries an intact and functional agrocinnopine synthase gene close to its left border. TA/TL sequence comparison shows that the biotype I TL region still carries a 5'-deleted *acs* gene, strongly indicating that this gene was originally part of the TL region and belongs to the "common DNA" region of octopine and nopaline Ti plasmids. Tm4 and C58C1 (pTiTm4) remove agrocinnopine A from the medium indicating that pTiTm4 also carries agrocinnopine uptake genes. In spite of this, Tm4 and related strains are resistant against agrocinn 84. Two o/c Ti plasmids that are closely related to pTiTm4, pTiHm1, and pTiAB3, have a mutated *acs* gene; whereas Hm1 can still take up agrocinnopine A, AB3 cannot. These results yield new insights in the evolution of octopine, nopaline, and o/c strains.

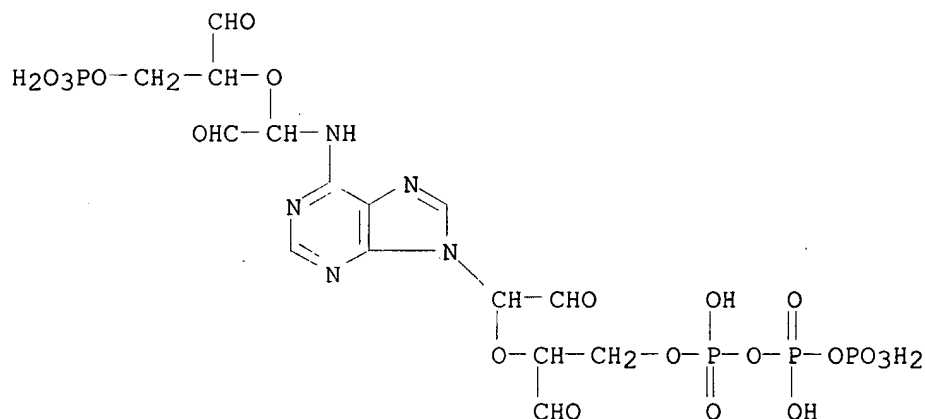
L5 ANSWER 130 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 56475-05-9 REGISTRY

CN Triphosphoric acid, P-[2-[1-[6-[1-[1-formyl-2-(phosphonoxy)ethoxy]-2-oxoethyl]amino]-9H-purin-9-yl]-2-oxoethoxy]-3-oxopropyl] ester, stereoisomer (9CI) (CA INDEX NAME)

MF C15 H21 N5 O20 P4

LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)

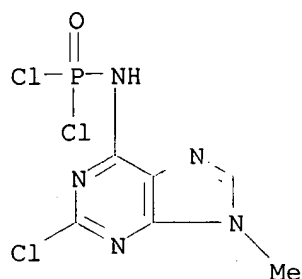
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 83:93004 Stereochemical course of the adenosine triphosphate phosphoribosyltransferase reaction in histidine biosynthesis. Chelsky, Daniel; Parsons, Stanley M. (Dep. Chem., Univ. California, Santa Barbara, Calif., USA). *J. Biol. Chem.*, 250(14), 5669-73 (English) 1975. CODEN: JBCHA3.

AB The product of the 1st reaction in histidine biosynthesis was shown by optical rotation measurements on 3 derivs. to have inverted, .beta. stereochem. at the newly formed bond. This is in contrast to .alpha. linkage expected on the basis of previously obsd. exchange, specificity, and covalent intermediate phenomena. The postulated double displacement mechanism for ATP phosphoribosyltransferase (EC 2.4.2.17) must be modified to account for the product stereochem.

Searched by: Mary Hale 308-4258 CM-1 1E01

L5 ANSWER 131 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 36615-79-9 REGISTRY
 CN Phosphoramidic dichloride, (2-chloro-9-methyl-9H-purin-6-yl)- (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C6 H5 Cl3 N5 O P
 LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER
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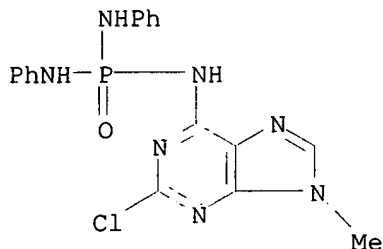


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 77:5431 Syntheses of purines. XXVI. 6-Bis(ethylenimido)phosphamidopurines. Korsunskii, V. S.; Chaman, E. S.; Golovchinskaya, E. S. (Vses. Nauchno-Issled. Khim.-Farm. Inst. im. Ordzhonikidze, Moscow, USSR). Khim.-Farm. Zh., 6(3), 10-14 (Russian) 1972. CODEN: KHFZAN.
 GI For diagram(s), see printed CA Issue.
 AB ,6-Dichloro-7- and -9-methylpurine reacted with NH₃ to give 2-chloro-7- and -9-methyladenine (I), resp., which gave methyladenines [II and III, resp., R = H, N(CH₂CH:CH₂)₂, piperidino, morpholino; R₁ = H] with III and red P or the corresponding secondary amine. II and III (R₁ = H) were converted to the title compds. [II and III, R₁ = bis(ethylenimido)phosphoro] by treatment with POCl₃ and then ethylenimine. I gave III [R = Cl, R₁ = bis(ethylenimido)phosphoro] with PCl₅ and then HCO₂H. The products had antitumor activity in mice and rats.

L5 ANSWER 132 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 36615-78-8 REGISTRY
 CN Phosphoric triamide, N-(2-chloro-9-methyl-9H-purin-6-yl)-N',N''-diphenyl- (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C18 H17 Cl N7 O P
 LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER
 (*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 77:5431 Syntheses of purines. XXVI. 6-Bis(ethylenimido)phosphamidopurines. Korsunskii, V. S.; Chaman, E. S.; Golovchinskaya, E. S. (Vses. Nauchno-Issled. Khim.-Farm. Inst. im. Ordzhonikidze, Moscow, USSR). Khim.-Farm. Zh., 6(3), 10-14 (Russian) 1972. CODEN: KHFZAN.

GI For diagram(s), see printed CA Issue.

AB ,6-Dichloro-7- and -9-methylpurine reacted with NH₃ to give 2-chloro-7- and -9-methyladenine (I), resp., which gave methyladenines [II and III, resp., R = H, N(CH₂CH:CH₂)₂, piperidino, morpholino; R₁ = H] with III and red P or the corresponding secondary amine. II and III (R₁ = H) were converted to the title compds. [II and III, R₁ = bis(ethylenimido)phosphoro] by treatment with POCl₃ and then ethylenimine. I gave III [R = Cl, R₁ = bis(ethylenimido)phosphoro] with PCl₅ and then HCO₂H. The products had antitumor activity in mice and rats.

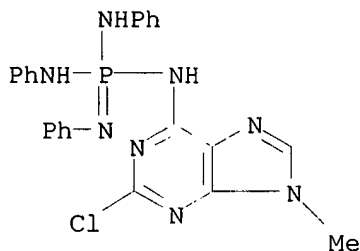
L5 ANSWER 133 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 36615-75-5 REGISTRY

CN Phosphorimidic triamide, N-(2-chloro-9-methyl-9H-purin-6-yl)-N',N'',N'''-triphenyl- (9CI) (CA INDEX NAME)

MF C24 H22 Cl N8 P

LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 77:5431 Syntheses of purines. XXVI. 6-Bis(ethylenimido)phosphamidopurines. Korsunskii, V. S.; Chaman, E. S.; Golovchinskaya, E. S. (Vses. Nauchno-Issled. Khim.-Farm. Inst. im.

Ordzhonikidze, Moscow, USSR). Khim.-Farm. Zh., 6(3), 10-14 (Russian) 1972. CODEN: KHFZAN.

GI For diagram(s), see printed CA Issue.

AB ,6-Dichloro-7- and -9-methylpurine reacted with NH₃ to give 2-chloro-7- and -9-methyladenine (I), resp., which gave methyladenines [II and III, resp., R = H, N(CH₂CH:CH₂)₂, piperidino, morpholino; R₁ = H] with III and red P or the corresponding secondary amine. II and III (R₁ = H) were converted to the title compds. [II and III, R₁ = bis(ethylenimido)phosphoro] by treatment with POCl₃ and then ethylenimine. I gave III [R = Cl, R₁ = bis(ethylenimido)phosphoro] with PCl₅ and then HCO₂H. The products had antitumor activity in mice and rats.

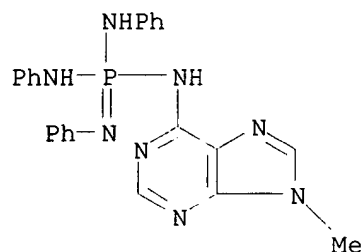
L5 ANSWER 134 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 36615-74-4 REGISTRY

CN Phosphorimidic triamide, N-(9-methyl-9H-purin-6-yl)-N',N'',N'''-triphenyl- (9CI) (CA INDEX NAME)

MF C24 H23 N8 P

LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 77:5431 Syntheses of purines. XXVI. 6-Bis(ethylenimido)phosphamidopurines. Korsunskii, V. S.; Chaman, E. S.; Golovchinskaya, E. S. (Vses. Nauchno-Issled. Khim.-Farm. Inst. im. Ordzhonikidze, Moscow, USSR). Khim.-Farm. Zh., 6(3), 10-14 (Russian) 1972. CODEN: KHFZAN.

GI For diagram(s), see printed CA Issue.

AB ,6-Dichloro-7- and -9-methylpurine reacted with NH₃ to give 2-chloro-7- and -9-methyladenine (I), resp., which gave methyladenines [II and III, resp., R = H, N(CH₂CH:CH₂)₂, piperidino, morpholino; R₁ = H] with III and red P or the corresponding secondary amine. II and III (R₁ = H) were converted to the title compds. [II and III, R₁ = bis(ethylenimido)phosphoro] by treatment with POCl₃ and then ethylenimine. I gave III [R = Cl, R₁ = bis(ethylenimido)phosphoro] with PCl₅ and then HCO₂H. The products had antitumor activity in mice and rats.

L5 ANSWER 135 OF 140 REGISTRY COPYRIGHT 2002 ACS

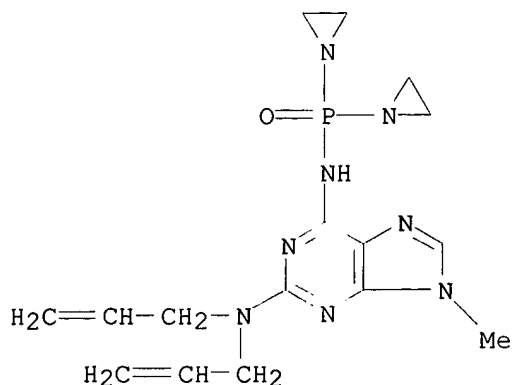
RN 36615-73-3 REGISTRY

CN Phosphinic amide, P,P-bis(1-aziridiny)-N-[2-(di-2-propenylamino)-9-methyl-9H-purin-6-yl]- (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C16 H23 N8 O P

LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 77:5431 Syntheses of purines. XXVI. 6-Bis(ethylenimido)phosphamidopurines. Korsunskii, V. S.; Chaman, E. S.; Golovchinskaya, E. S. (Vses. Nauchno-Issled. Khim.-Farm. Inst. im. Ordzhonikidze, Moscow, USSR). Khim.-Farm. Zh., 6(3), 10-14 (Russian) 1972. CODEN: KHFZAN.

GI For diagram(s), see printed CA Issue.

AB ,6-Dichloro-7- and -9-methylpurine reacted with NH₃ to give 2-chloro-7- and -9-methyladenine (I), resp., which gave methyladenines [II and III, resp.; R = H, N(CH₂CH:CH₂)₂, piperidino, morpholino; R₁ = H] with III and red P or the corresponding secondary amine. II and III (R₁ = H) were converted to the title compds. [II and III, R₁ = bis(ethylenimido)phosphoro] by treatment with POCl₃ and then ethylenimine. I gave III [R = Cl, R₁ = bis(ethylenimido)phosphoro] with PC15 and then HCO₂H. The products had antitumor activity in mice and rats.

L5 ANSWER 136 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 32600-71-8 REGISTRY

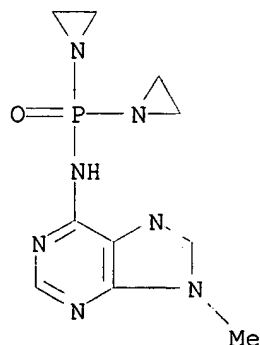
CN Phosphinic amide, P,P-bis(1-aziridinyl)-N-(9-methyl-9H-purin-6-yl)- (8CI, 9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C10 H14 N7 O P

LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER

(*File contains numerically searchable property data)

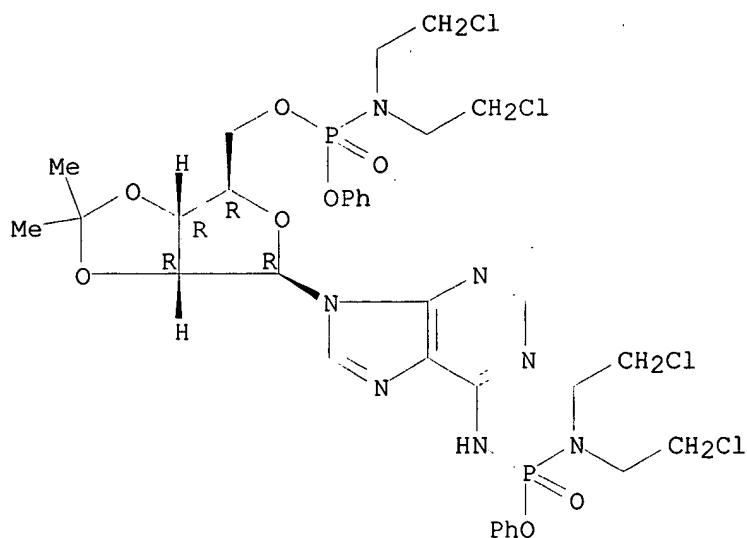


****PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT****

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

- REFERENCE 1: 77:5431 Syntheses of purines. XXVI. 6-Bis(ethylenimido)phosphamidopurines. Korsunskii, V. S.; Chaman, E. S.; Golovchinskaya, E. S. (Vses. Nauchno-Issled. Khim.-Farm. Inst. im. Ordzhonikidze, Moscow, USSR). Khim.-Farm. Zh., 6(3), 10-14 (Russian) 1972. CODEN: KHFZAN.
- GI For diagram(s), see printed CA Issue.
- AB ,6-Dichloro-7- and -9-methylpurine reacted with NH₃ to give 2-chloro-7- and -9-methyladenine (I), resp., which gave methyladenines [II and III, resp., R = H, N(CH₂CH:CH₂)₂, piperidino, morpholino; R₁ = H] with III and red P or the corresponding secondary amine. II and III (R₁ = H) were converted to the title compds. [II and III, R₁ = bis(ethylenimido)phosphoro] by treatment with POCl₃ and then ethylenimine. I gave III [R = Cl, R₁ = bis(ethylenimido)phosphoro] with PCl₅ and then HCO₂H. The products had antitumor activity in mice and rats.
- REFERENCE 2: 75:35943 Diethylenimidophosphamido derivatives of purine. Korsunskii, V. S.; Golovchinskaya, E. S. (Vses. Nauchno-Issled. Khim.-Farm. Inst., Moscow, USSR). Puti Sin. Izyskaniya Protivopukholevykh Prep., Volume Date 1968, No. 3, 323-9 (Russian) 1970. CODEN: PSIPA4.
- AB Chlorination with Cl of caffeine (I) and isocaffeine (II) gave the 8-trichloromethyl derivs. of I and II. The next Cl atom entered the 7-Me of I or the 3-Me of II. The former deriv. was hydrolyzed to theophylline and the latter to 1,9-dimethylxanthine. 7-Methyl- or 9-methyladenine (III or IV, resp.) was treated with POCl₃ and the resulting dichloride of amidophosphoric acid treated with ethylenimine and HCl acceptors to give both 6-diethylenimidophosphoramido derivs. of III and IV, which were tested against sarcomas 45 and 37, and carcinoma NK. The growth retardations were 60-80, 49-56, and 37-48%, resp. The activity of the III deriv. was slightly higher than that of IV. IV was also prepd. from trihydroxypurine (ureic acid), via 1,9-dimethylxanthine and the 9-Me deriv. of 2,6-dichloropurine (V). Similarly, III was prepd. from theobromine via the 7-Me deriv. of V.
- L5 ANSWER 137 OF 140 REGISTRY COPYRIGHT 2002 ACS
- RN 13190-67-5 REGISTRY
- CN Phosphorodiamidic acid, N,N-bis(2-chloroethyl)-N'-[9-(2,3-O-isopropylidene-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, phenyl ester, phenyl bis(2-chloroethyl)phosphoramidate (ester) (8CI) (CA INDEX NAME)
- OTHER CA INDEX NAMES:
- CN Adenosine, N-[[bis(2-chloroethyl)amino]phenoxyphosphinyl]-2',3'-O-isopropylidene-, 5'-[phenyl bis(2-chloroethyl)phosphoramidate]
- CN Phosphorodiamidic acid, N,N-bis(2-chloroethyl)-N'-[9-(2,3-O-isopropylidene-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, phenyl ester, phenyl bis(2-chloroethyl)phosphoramidate (7CI)
- FS STEREOSEARCH
- MF C33 H41 Cl4 N7 O8 P2
- LC STN Files: BEILSTEIN*, CAOLD
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L5 ANSWER 138 OF 140 REGISTRY COPYRIGHT 2002 ACS

RN 10154-11-7 REGISTRY

CN Phosphinic amide, P,P-bis(1-aziridinyl)-N-(2-chloro-9-methyl-9H-purin-6-yl)- (7CI, 8CI, 9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 9H-Purine, 6-[[bis(1-aziridinyl)phosphinyl]amino]-2-chloro-9-methyl-

OTHER NAMES:

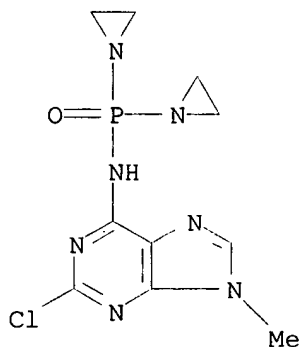
CN 2-Chloro-6-(diethyleniminophosphamido)-9-methylpurine

FS 3D CONCORD

MF C10 H13 Cl N7 O P

LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, TOXCENTER

(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1967 TO DATE)

3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

Searched by: Mary Hale 308-4258 CM-1 1E01

REFERENCE 1: 79:133343 Mutability of chromosomes of embryonic human cells induced by some analogs of nitrogenous bases. Lekevicius, R.; Kalpokaite, Z.; Jasinskaite, R. (Vil'nyus. Gos. Univ., Vilnius, USSR). Sin. Izuch. Fiziol. Aktiv. Veshchestv, Mater. Konf., 73-4. Vil'nyus. Gos. Univ.: Vilnyus, USSR. (Russian) 1971. CODEN: 26YYAS.

AB Autoradiog. studies with 3T-labeled thymidine showed that 2-chloro-6-diethyleniminophosphamido-9-methylpurine [10154-11-7], 2-chloro-6-bis(.beta.-chloroethyl)aminomethyl-9-methylpurine [13726-50-6], 2-dimethylamino-6-diethyleniminophosphamido-7-methylpurine [42061-52-9], or 2-chloro-6-dimethyleniminophosphamido-7-methylpurine [42061-53-0] increased by 4-6 times the total no. of mutations developing in the chromosomes of 2-month human embryo cells. The proportion of induced mutation types was the same as the proportion obsd. during spontaneous mutagenesis. All 4 compds. increased the length of the mitotic cycle by prolonging the G1 and S stages.

REFERENCE 2: 77:5431 Syntheses of purines. XXVI. 6-Bis(ethylenimido)phosphamidopurines. Korsunskii, V. S.; Chaman, E. S.; Golovchinskaya, E. S. (Vses. Nauchno-Issled. Khim.-Farm. Inst. im. Ordzhonikidze, Moscow, USSR). Khim.-Farm. Zh., 6(3), 10-14 (Russian) 1972. CODEN: KHFZAN.

GI For diagram(s), see printed CA Issue.

AB ,6-Dichloro-7- and -9-methylpurine reacted with NH3 to give 2-chloro-7- and -9-methyladenine (I), resp., which gave methyladenines [II and III, resp., R = H, N(CH2CH:CH2)2, piperidino, morpholino; R1 = H] with III and red P or the corresponding secondary amine. II and III (R1 = H) were converted to the title compds. [II and III, R1 = bis(ethylenimido)phosphoro] by treatment with POCl3 and then ethylenimine. I gave III [R = Cl, R1 = bis(ethylenimido)phosphoro] with PCl5 and then HCO2H. The products had antitumor activity in mice and rats.

REFERENCE 3: 67:20237 Analysis of the cytogenetic and cytostatic effects of 2-chloro-6-(diethyleniminophosphamido)-9-methylpurine on the cells of the Ehrlich carcinoma. Dubinin, N. P.; Lekevicius, R. (Inst. Gen. Genet., Moscow, USSR). Genetika (Moscow) (2), 3-11 (Russian) 1967. CODEN: GNKAA5.

AB A cytogenetic effect of a single dose of 2-chloro-6-(diethyleniminophosphamido)-9-methylpurine applied at 10-5M is described. This effect continued through several cell generations both on normal human tissue culture and on Ehrlich ascites tumor cell. The decrease of mitotic activity in subsequent generations was observed in normal cells only. The frequency of chromosomal mutation at this concn. was trebled. Rearrangements of chromosomes do not affect the redn. of mitotic activity.

L5 ANSWER 139 OF 140 REGISTRY COPYRIGHT 2002 ACS

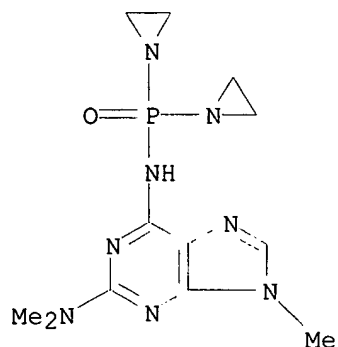
RN 3861-04-9 REGISTRY

CN Phosphinic amide, P,P-bis(1-aziridinyI)-N-[2-(dimethylamino)-9-methyl-9H-purin-6-yl]- (8CI, 9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C12 H19 N8 O P

LC STN Files: CAOLD

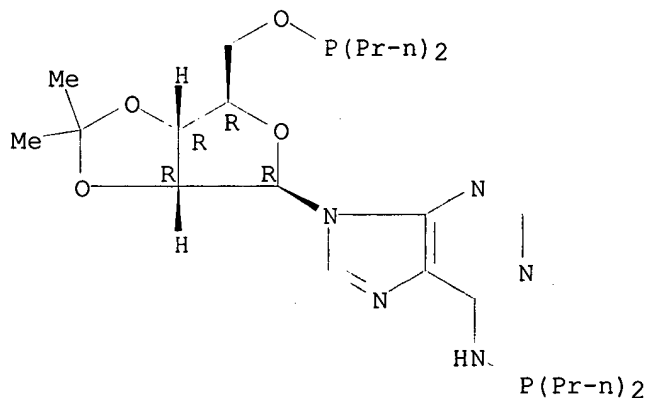


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L5 ANSWER 140 OF 140 REGISTRY COPYRIGHT 2002 ACS
 RN 3056-38-0 REGISTRY
 CN Adenosine, N-[9-(O-isopropylidene-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-
 P,P-dipropyl-, 5'-dipropylphosphinite (8CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C25 H43 N5 O4 P2
 LC STN Files: CAOLD

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> fil caol;s 15
 COST IN U.S. DOLLARS
 FULL ESTIMATED COST

SINCE FILE ENTRY	TOTAL SESSION
675.85	676.06

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE ENTRY	TOTAL SESSION
-75.52	-75.52

CA SUBSCRIBER PRICE

FILE 'CAOLD' ENTERED AT 13:32:56 ON 21 JUN 2002

Searched by: Mary Hale 308-4258 CM-1 1E01

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FILE LAST UPDATED: 01 May 1997 (19970501/UP)

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This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

L6 6 L5

=> d 1-6

L6 ANSWER 1 OF 6 CAOLD COPYRIGHT 2002 ACS
AN CA65:13809c CAOLD
TI synthesis of oligodeoxynucleotides with terminal 5' -phosphate groups
AU Eckstein, Fritz
IT 2642-45-7 13190-60-8 13190-66-4 **13190-67-5** 13190-69-7
13190-72-2 13190-75-5 13492-95-0 13972-98-0 14952-66-0 15664-25-2

L6 ANSWER 2 OF 6 CAOLD COPYRIGHT 2002 ACS
AN CA65:2863b CAOLD
TI induction of tryptophan pyrrolase in the liver of the rat treated with nicotinamide
AU Pallini, V.; Vasconetto, C.; Ricci, C.
IT **10154-11-7**

L6 ANSWER 3 OF 6 CAOLD COPYRIGHT 2002 ACS
AN CA64:20257c CAOLD
TI mutagenic activity of N-substituted ethylenimines
AU Bartoshevich, Yu. E.; Kostyanovskii, R. G.
IT 460-07-1 503-12-8 696-18-4 738-99-8 882-58-6 1074-42-6
1078-79-1 1135-06-4 1497-82-1 1497-83-2 1523-27-9 1523-28-0
1593-49-3 2407-60-5 2541-35-7 3029-67-2 3408-52-4 3795-89-9
3795-90-2 3795-91-3 3795-93-5 3795-94-6 3795-95-7 3795-98-0
3795-99-1 3796-00-7 **3861-04-9** 3861-05-0 3861-06-1
3974-84-3 3974-85-4 3974-91-2 4025-27-8 4025-28-9 4025-30-3
4025-31-4 4025-41-6 4025-42-7 4921-46-4 6999-33-3 7410-92-6
7410-93-7 7410-95-9 7410-97-1 7410-98-2 7411-02-1 7411-04-3
7417-97-2 7439-09-0 7444-90-8

L6 ANSWER 4 OF 6 CAOLD COPYRIGHT 2002 ACS
AN CA62:626f CAOLD
TI 2'-O-(.alpha.-ethoxyethyl)-5'-O-acetyluridine 3'-phosphate, a key intermediate for oligonucleotide synthesis
AU Chladek, Stanislav; Smrt, J.
IT 3245-32-7 **101837-90-5**

L6 ANSWER 5 OF 6 CAOLD COPYRIGHT 2002 ACS
AN CA62:626e CAOLD
TI synthesis of phosphonites and phosphinites of nucleosides
AU Nifant'ev, E. E.; Markov, S. M.; Tuseev, A. P.

Searched by: Mary Hale 308-4258 CM-1 1E01

IT 3056-38-0 5286-68-0

L6 ANSWER 6 OF 6 CAOLD COPYRIGHT 2002 ACS
AN CA62:26d CAOLD
TI fluorometric detn. of U with Rhodamine B
AU Andersen, Neil R.; Hercules, D. M.
IT 3056-38-0

=> fil hcap;s l6

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
3.80	679.86

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE	TOTAL
ENTRY	SESSION
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FILE COVERS 1907 - 21 Jun 2002 VOL 136 ISS 25
FILE LAST UPDATED: 19 Jun 2002 (20020619/ED)

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CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

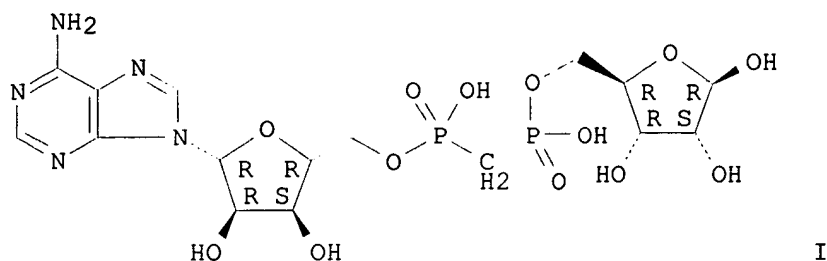
L7 77 L5

=> d 11-77 cbib abs hitstr

L7 ANSWER 11 OF 77 HCAPLUS COPYRIGHT 2002 ACS
1996:600877 Document No. 125:301465 Synthesis of methylenebis(phosphonate) analogs of ADP-Ribose. Pankiewicz, Krzysztof W.; Lesiak, Krystyna; Zatorski, Andrzej; Watanabe, Kyoichi A. (OncorPharm, Inc., Gaithersburg, MD, 20877, USA). Collect. Czech. Chem. Commun., 61(Spec. Issue), S92-S95 (English) 1996. CODEN: CCCCAK. ISSN: 0010-0765.

GI

Searched by: Mary Hale 308-4258 CM-1 1E01



AB An efficient synthesis of analogs of ADP-ribose contg. a methylene group instead of pyrophosphate oxygen is described. A target compd. was the ribose analog I. Formation of a cADP-ribose analog and cIDP-ribose analogs, in which N1-ribose was replaced by butanol, was also reported.

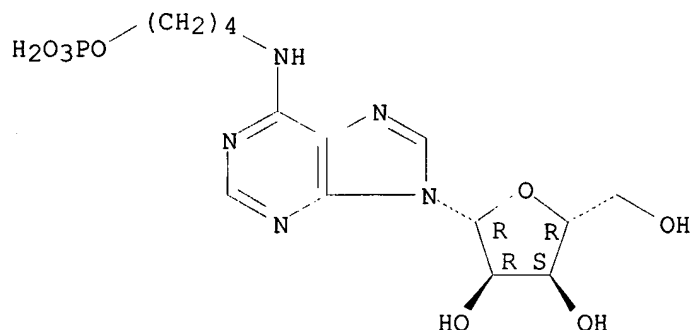
IT **182950-56-7P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of methylenebis(phosphonate) analogs of ADP-Ribose)

RN 182950-56-7 HCAPLUS

CN Adenosine, N-[4-(phosphonoxy)butyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 12 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1996:333885 Document No. 125:2931 Spontaneous transfer of the Ti plasmid of *Agrobacterium tumefaciens* and the nopaline catabolism plasmid of *A. radiobacter* strain K84 in crown gall tissue. Vicedo, Begonya; Lopez, Maria Jose; Asins, Maria Jose; Lopez, Maria M. (Instituto Valenciano de Investigaciones Agrarias, Moncada, 46113, Spain). *Phytopathology*, 86(5), 528-534 (English) 1996. CODEN: PHYTAJ. ISSN: 0031-949X.

AB Spontaneous transfer of the Ti plasmid from *Agrobacterium tumefaciens* to strain K84 of *A. radiobacter* was obsd. and studied for the first time in an expt. on biol. control of crown gall. This transfer was detected in a tumor from a K84-treated plant grown in soil inoculated with a nopaline strain of *A. tumefaciens* biovar 1 sensitive to agrocin 84. The transconjugant strain was virulent and produced agrocin 84. Southern blot hybridization anal. with several probes (T-DNA and right adjacent regions and vir genes) showed important changes at the Ti plasmid, suggesting that recombination between Ti plasmid and pAtK84b in K84 could have happened, resulting in a new Ti plasmid. Transfer of both plasmids of strain K84, pAtK84b and pAgK84, responsible for nopaline catabolism and agrocin 84 prodn., resp., to *A. tumefaciens* also was detected in isolates from the same tumor. Southern blot hybridization of plasmids from one of these avirulent isolates with a nopaline plasmid-specific probe of strain K84 indicated there was a replacement of Ti plasmid by pAtK84b in *A.*

IT 59111-78-3, Agrocin 84
RL: MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)

RN 59111-78-3 HCAPLUS

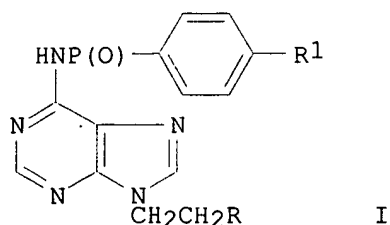
Absolute stereochemistry.

The chemical structure shows a complex molecule with several functional groups and rings. On the left, a pyrimidine ring is connected to a furanose ring via a C-glycosidic bond. The pyrimidine ring has a hydroxyl group at the 6-position and a thioether linkage at the 5-position. The furanose ring has a hydroxyl group at the 2-position and a thioether linkage at the 3-position. The thioether linkage connects the furanose ring to a thioester group, which is further connected to a carboxylic acid group. The carboxylic acid group is shown as a thioester, with a sulfur atom double-bonded to a carbonyl group and a hydroxyl group attached to the sulfur atom. The entire molecule is labeled with 'R' and 'S' stereochemistry at various chiral centers.

$$\begin{array}{c} \text{OH} \\ | \\ \text{R} \end{array} \text{Pr-i}$$

GI

Searched by: Mary Hale 308-4258 CM-1 1E01



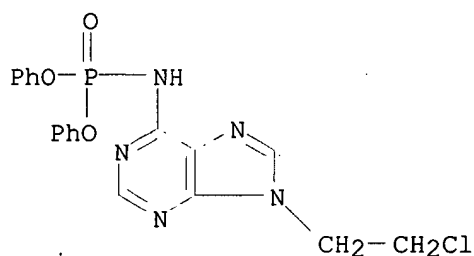
AB Phosphorylated adenines I [R = Cl; R1 = H, Me] were prepd. from 9-(2-hydroxyethyl)adenine (II) by reaction with ClP(O)(OC6H4R1-4)2. I [R = Cl] were converted to I [R = N3, pyridylamino]. II was also converted to phosphate esters and phosphonates and phosphates of aniline and 4-aminopyridine were also prepd.

IT 167780-54-3P 167780-55-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. of phosphorylated adenine derivs.)

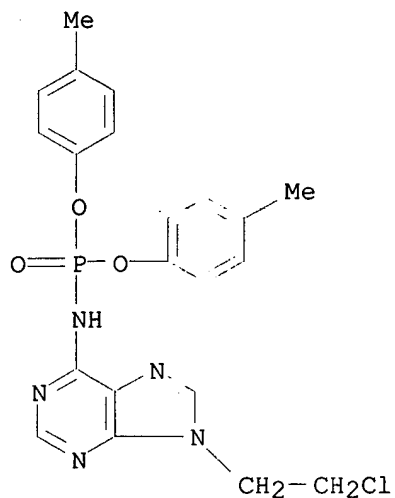
RN 167780-54-3 HCAPLUS

CN Phosphoramidic acid, [9-(2-chloroethyl)-9H-purin-6-yl]-, diphenyl ester (9CI) (CA INDEX NAME)



RN 167780-55-4 HCAPLUS

CN Phosphoramidic acid, [9-(2-chloroethyl)-9H-purin-6-yl]-, bis(4-methylphenyl) ester (9CI) (CA INDEX NAME)

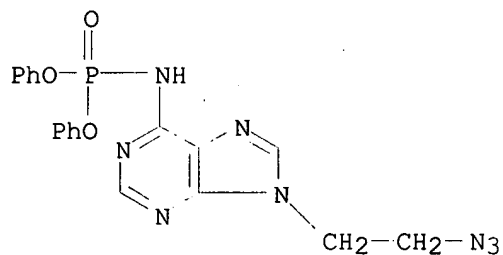


IT 167780-56-5P 167780-57-6P 167780-58-7P
167780-59-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of phosphorylated adenine derivs.)

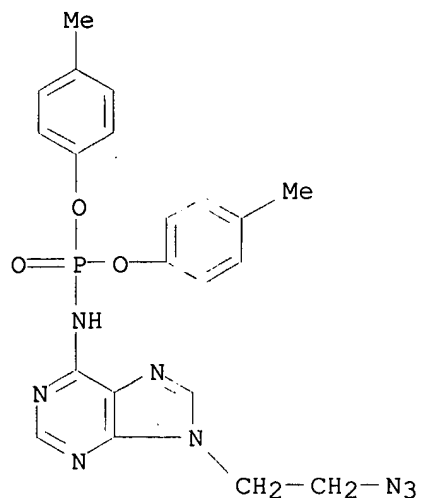
RN 167780-56-5 HCAPLUS

CN Phosphoramidic acid, [9-(2-azidoethyl)-9H-purin-6-yl]-, diphenyl ester
(9CI) (CA INDEX NAME)



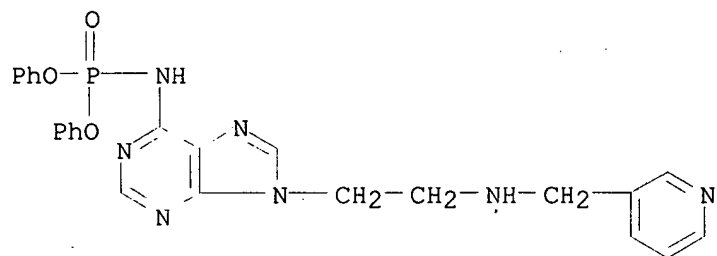
RN 167780-57-6 HCAPLUS

CN Phosphoramidic acid, [9-(2-azidoethyl)-9H-purin-6-yl]-,
bis(4-methylphenyl) ester (9CI) (CA INDEX NAME)



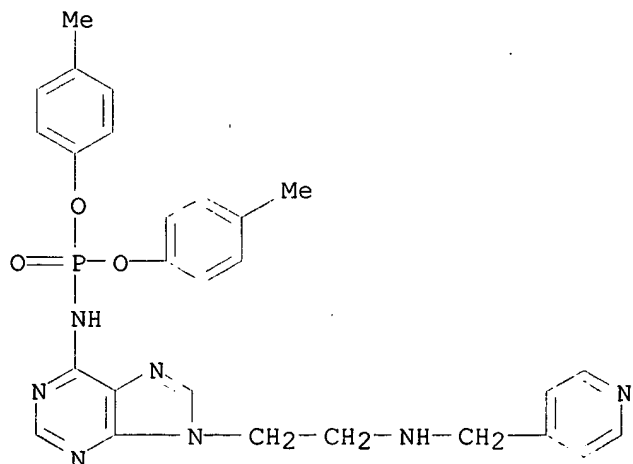
RN 167780-58-7 HCAPLUS

CN Phosphoramidic acid, [9-[2-[(3-pyridinylmethyl)amino]ethyl]-9H-purin-6-yl]-, diphenyl ester (9CI) (CA INDEX NAME)



RN 167780-59-8 HCAPLUS

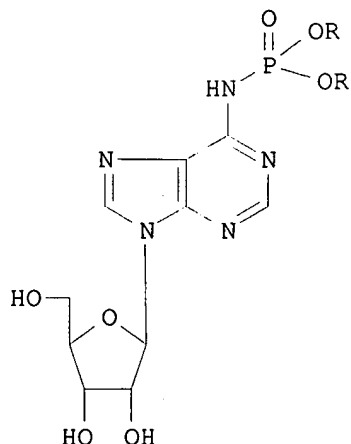
CN Phosphoramidic acid, [9-[2-[(4-pyridinylmethyl)amino]ethyl]-9H-purin-6-yl]-, bis(4-methylphenyl) ester (9CI) (CA INDEX NAME)



L7 ANSWER 14 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1995:130749 Document No. 122:214406 Synthesis and Properties of
N-Phosphorylated Ribonucleosides. Wada, Takeshi; Moriguchi, Tomohisa;
Sekine, Mitsuo (Faculty of Bioscience and Biotechnology, Tokyo Institute
of Technology, Yokohama, 227, Japan). J. Am. Chem. Soc., 116(22), 9901-11
(English) 1994. CODEN: JACSAT. ISSN: 0002-7863.

GI



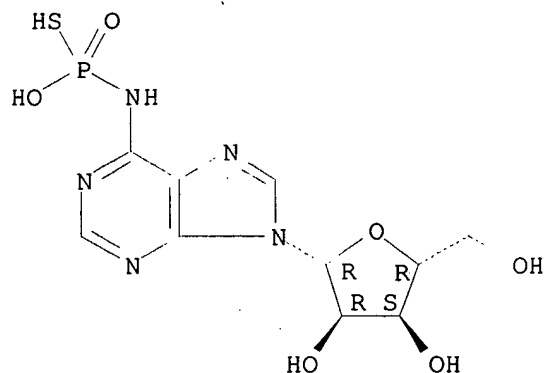
AB A new class of phosphorylated nucleosides,, e.g. I (R = Na, Et), were synthesized in good yields via phosphitylation of the amino group of appropriately protected adenosine derivs. In a similar manner, cytidine 4-N-phosphoramidate (4-N-CMP), guanosine 2-N-phosphoramidate (2-N-GMP), and their di-Et ester derivs. were synthesized. These new compds. were characterized by ¹H, ¹³C, and ³¹P NMR, UV, CD, IR, electrophoresis, and mass spectroscopy. The conformation and water soly. of these N-phosphorylated ribonucleoside derivs. have been studied in detail.

IT **161879-75-0P 161879-76-1P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn., conformation, and water soly. of N-phosphorylated nucleosides)

RN 161879-75-0 HCAPLUS

CN Phosphoramidothioic acid, (9-.beta.-D-ribofuranosyl-9H-purin-6-yl)-,
disodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

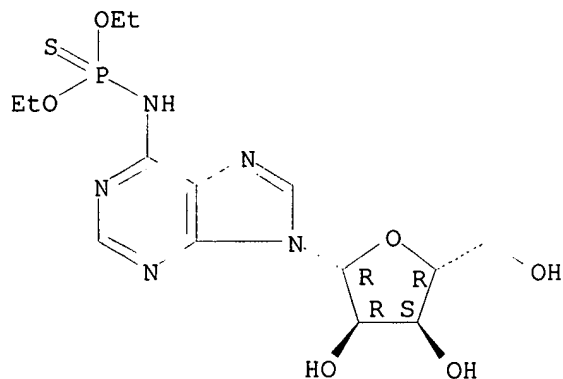


●2 Na

RN 161879-76-1 HCAPLUS

CN Phosphoramidothioic acid, (9-.beta.-D-ribofuranosyl-9H-purin-6-yl)-, O,O-diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 154534-46-0P 154971-65-0P 154971-69-4P

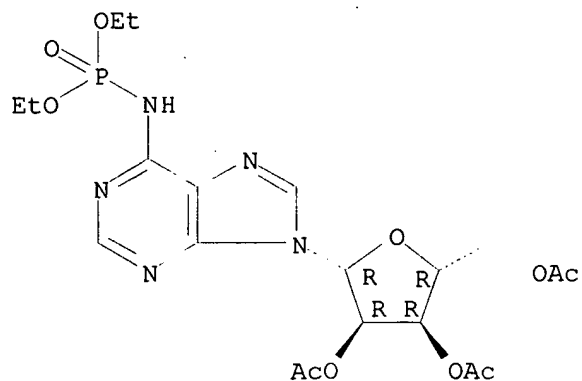
154986-10-4P 161879-73-8P 161879-74-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn., conformation, and water soly. of N-phosphorylated nucleosides)

RN 154534-46-0 HCAPLUS

CN Phosphoramidic acid, [9-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, diethyl ester (9CI) (CA INDEX NAME)

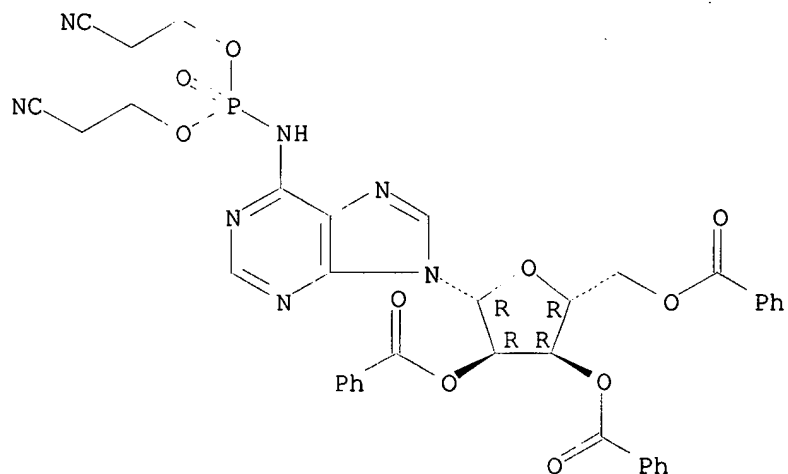
Absolute stereochemistry.



RN 154971-65-0 HCAPLUS

CN Phosphoramidic acid, [9-(2,3,5-tri-O-benzoyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, bis(2-cyanoethyl) ester (9CI) (CA INDEX NAME)

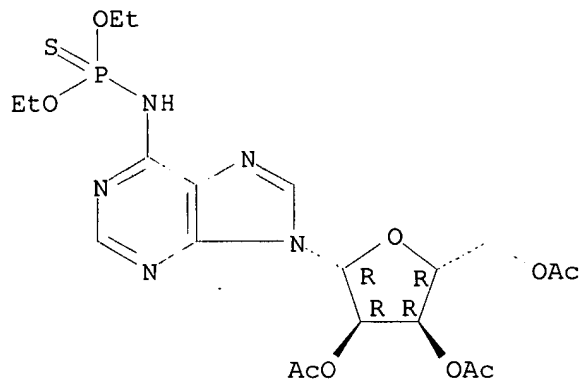
Absolute stereochemistry.



RN 154971-69-4 HCAPLUS

CN Phosphoramidothioic acid, [9-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, O,O-diethyl ester (9CI) (CA INDEX NAME)

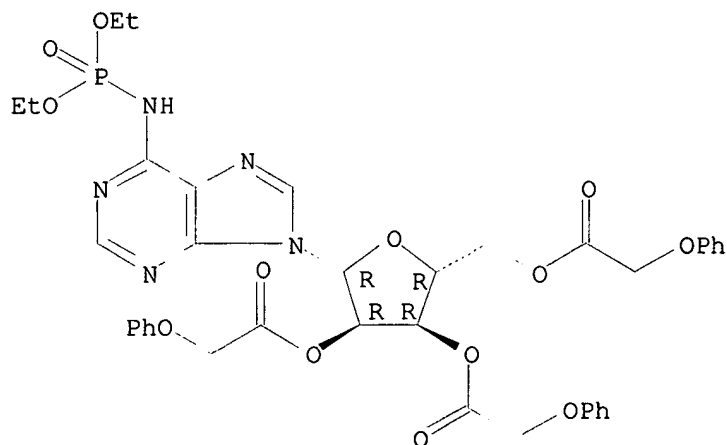
Absolute stereochemistry.



RN 154986-10-4 HCAPLUS

CN Phosphoramidic acid, [9-[2,3,5-tris-O-(phenoxyacetyl)-.beta.-D-ribofuranosyl]-9H-purin-6-yl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 161879-73-8 HCAPLUS

CN Phosphonamidic acid, P-1H-1,2,4-triazol-1-yl-N-[9-(2,3,5-tri-O-benzoyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

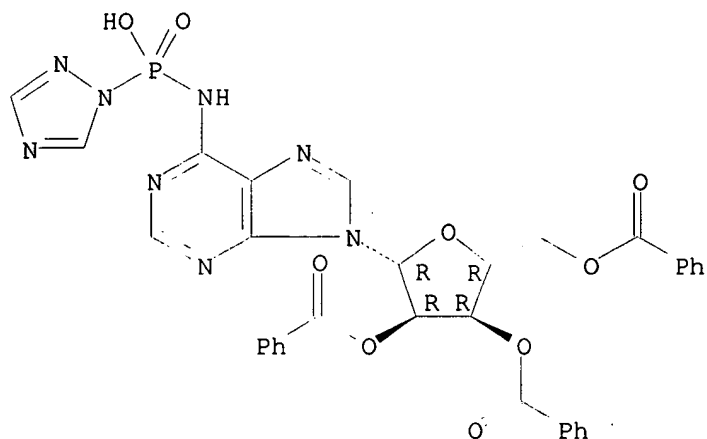
CM 1

CRN 161879-72-7

CMF C33 H27 N8 O9 P

CDES 5:B-D-RIBO

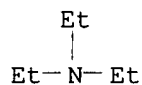
Absolute stereochemistry.



CM 2

CRN 121-44-8

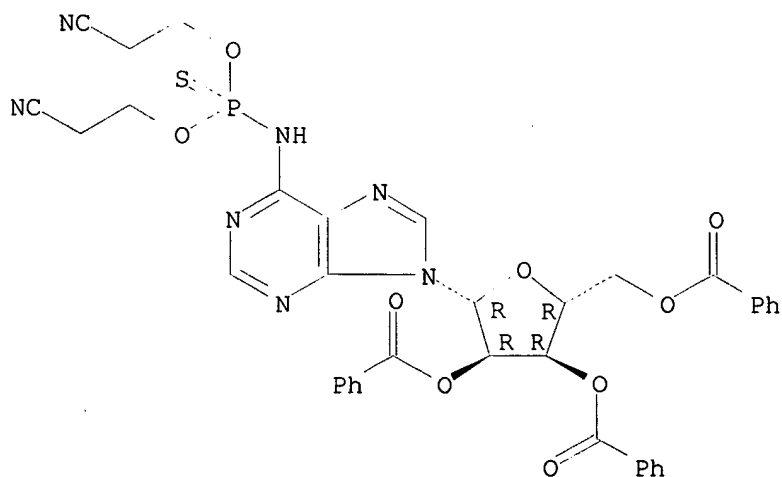
CMF C6 H15 N



RN 161879-74-9 HCAPLUS

CN Phosphoramidothioic acid, [9-(2,3,5-tri-O-benzoyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, O,O-bis(2-cyanoethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 154971-59-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn., conformation, and water soly. of N-phosphorylated nucleosides)

RN 154971-59-2 HCAPLUS

CN Phosphorodiamidic acid, (9-.beta.-D-ribofuranosyl-9H-purin-6-yl)-, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

Searched by: Mary Hale 308-4258 CM-1 1E01

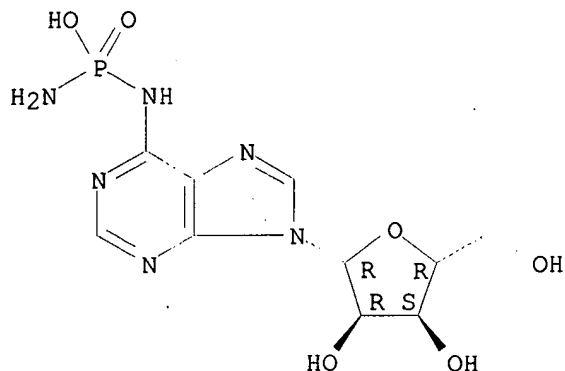
CM 1

CRN 154971-58-1

CMF C10 H15 N6 O6 P

CDES 5:B-D-RIBO

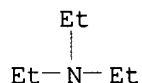
Absolute stereochemistry.



CM 2

CRN 121-44-8

CMF C6 H15 N



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1995:36308 Document No. 122:98736 Organization and expression of the genes on pAgK84 that encode production of agrocin 84. Wang, Chang-Lin; Farrand, Stephen K.; Hwang, Ingyu (Department of Plant Pathology, University of Illinois, Urbana, 61801, USA). Mol. Plant-Microbe Interact., 7(4), 472-81 (English) 1994. CODEN: MPMIEL. ISSN: 0894-0282.

AB Agrocin 84 biosynthesis genes located in a 21-kb segment of pAgK84 were characterized by mutagenesis with Tn3HoHol and complementation anal. Three overlapping fragments of the 21-kb segment, cloned into pRK415 or pLAFR6, were mutagenized with Tn3HoHol, and 94 independent insertions were mapped and oriented. A series of merodiploid strains, each contg. a Tn5 insertion in pAgK84 affecting agrocin 84 biosynthesis, and a clone contg. a Tn3HoHol insertion that blocks antibiotic prodn. in homogenotes were constructed to det. the no. of complementation groups involved in agrocin 84 biosynthesis. Five complementation groups were identified and named agnA through agnE. Anal. of lacZ fusions formed by the Tn3HoHol inserts indicated that all of the loci except agnD are transcribed in an anticlockwise direction. Insertions carried on clones and insertions marker-exchanged into pAgK84 had similar patterns of expression. The five agn loci were not expressed at significant levels in Escherichia coli DH5.alpha. grown in minimal or rich media. Levels of expression in Agrobacterium tumefaciens NT1 differed for each region; agnA was expressed at relatively high levels, agnC and agnE at intermediate levels, and agnB and agnD at very low levels. Similar patterns of expression were obsd. in minimal media, regardless of the carbon source, and at neutral and acidic

pHs. Expression levels were lower in cells grown in rich medium. The level of expression of each agn locus was not affected by the presence of other agn genes or by the presence or absence of the large nopaline plasmid pAtK84b, present in strain K84. Nor were the levels of expression influenced by the addn. of opines or root exudates to the culture media. All five agn loci were expressed at all growth stages, and expression reached max. levels during late exponential growth. The agn loci were expressed in planta, and the patterns of expression were similar to those seen in bacteria grown in vitro. The presence of pAtK84b did not affect agn expression in planta.

IT 59111-78-3, Agrocine 84

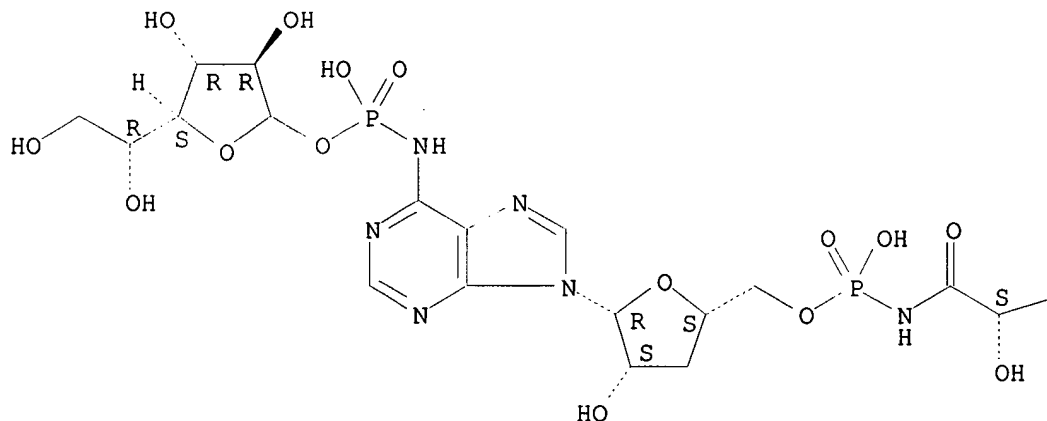
RL: BPR (Biological process); BIOL (Biological study); PROC (Process)
(organization and expression of genes on pAgK84 encode prodn. of
agrocine 84)

RN 59111-78-3 HCAPLUS

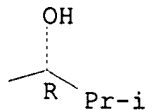
CN D-Glucosyl, 1-[hydrogen [9-[3-deoxy-5-O-[[[(4,5-dideoxy-4-methyl-D-threo-pentonyl)amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



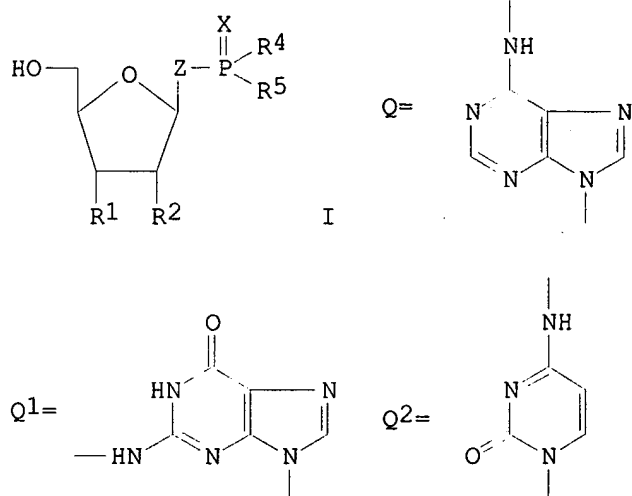
L7 ANSWER 16 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1994:324143 Document No. 120:324143 Preparation of nucleic acid-related
compounds. Sekine, Mitsuo; Wada, Takeshi (Wako Pure Chem Ind Ltd, Japan).
Jpn. Kokai Tokkyo Koho JP 06009681 A2 19940118 Heisei, 11 pp.

Searched by: Mary Hale 308-4258 CM-1 1E01

(Japanese). CODEN: JKXXAF. APPLICATION: JP 1993-76085 19930310.
 PRIORITY: JP 1992-88134 19920312.

GI



AB Nucleoside N-(thio)phosphoramidate derivs. [I; R1, R2 = H, OH; Z = Q - Q2; X = O, S, Se; R4, R5 = OH, NH2, (un)substituted C1-18 alkoxy or aryloxy], useful as pharmaceuticals, agrochems., and medical diagnostic agents (no data), are prepd. Thus, 1,2,4-1H-triazole was dissolved in acetone and reacted with P(O)Cl3 and Et3N at 0.degree. for 30 min and then with a soln. of 2',3',5'-tri-O-benzoyl-adenosine in MeCN to give 80% triethylammonium 2',3',5'-tri-O-benzoyl-adenosine-6-N-(triazolyl)phosphoramidate, which was treated with concd. aq. NH3-pyridine mixt. to give, after purifn. by anion exchange chromatog. using DEA cellulose and lyophilization, 83% triethylammonium adenosine-6-N-(amino)phosphoramidate.

IT **154971-61-6P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and ammonolysis-hydrolysis of)

RN 154971-61-6 HCAPLUS

CN Phosphonamidic acid, P-4H-1,2,4-triazol-4-yl-N-[9-(2,3,5-tri-O-benzoyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

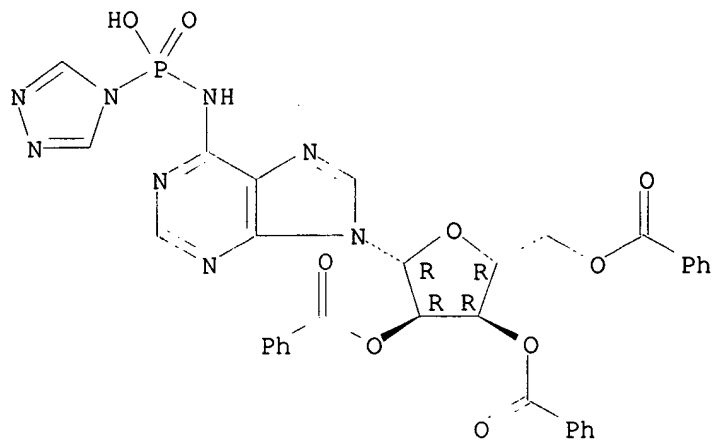
CM 1

CRN 154971-60-5

CMF C33 H27 N8 O9 P

CDES 5:B-D-RIBO

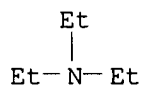
Absolute stereochemistry.



CM 2

CRN 121-44-8

CMF C6 H15 N



IT 154971-63-8P 154971-65-0P 154986-10-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and deprotection of)

RN 154971-63-8 HCAPLUS

CN Phosphoramidic acid, [9-(2,3,5-tri-O-benzoyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

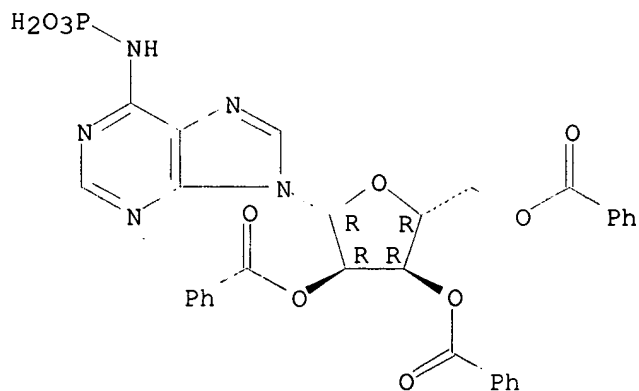
CM 1

CRN 154971-62-7

CMF C31 H26 N5 O10 P

CDES 5:B-D-RIBO

Absolute stereochemistry.

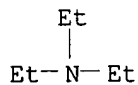


Searched by: Mary Hale 308-4258 CM-1 1E01

CM 2

CRN 121-44-8

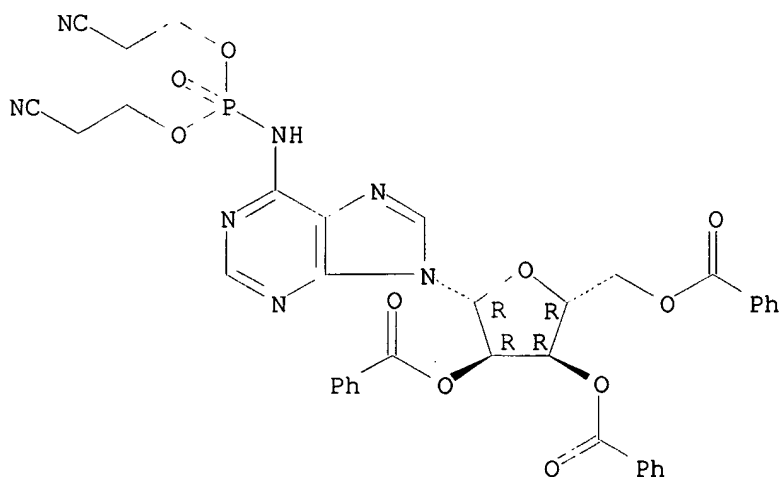
CMF C6 H15 N



RN 154971-65-0 HCAPLUS

CN Phosphoramidic acid, [9-(2,3,5-tri-O-benzoyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, bis(2-cyanoethyl) ester (9CI) (CA INDEX NAME)

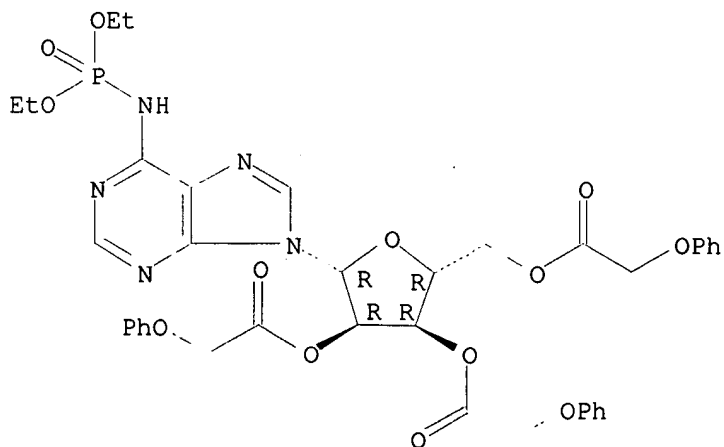
Absolute stereochemistry.



RN 154986-10-4 HCAPLUS

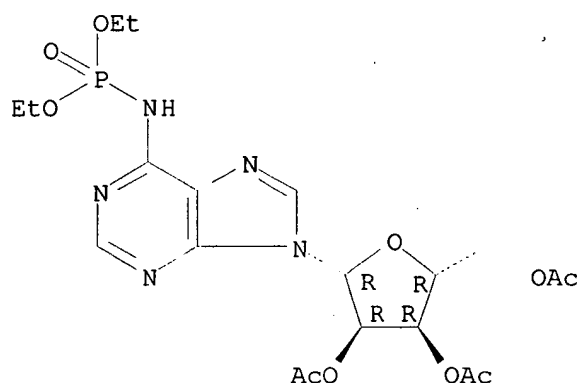
CN Phosphoramidic acid, [9-[2,3,5-tris-O-(phenoxyacetyl)-.beta.-D-ribofuranosyl]-9H-purin-6-yl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



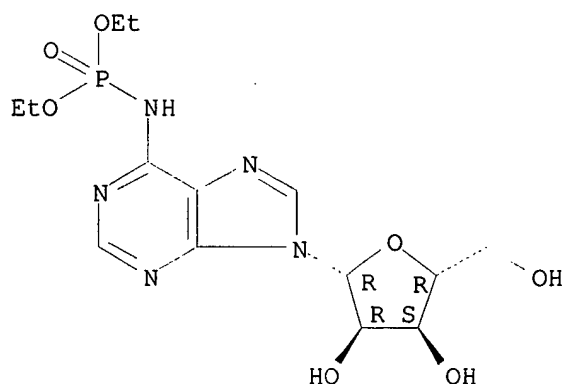
IT 154534-46-0P 154534-47-1P, Adenosine-6-N-(O,O-diethyl)phosphoramidate 154971-59-2P, Triethylammonium adenosine-6-N-(amino)phosphoramidate 154971-64-9P, Triethylammonium adenosine-6-N-phosphoramidate 154971-66-1P, Disodium adenosine-6-N-phosphoramidate 154971-67-2P 154971-69-4P
 RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of, as drug, agrochem., and medical diagnostic agent)
 RN 154534-46-0 HCAPLUS
 CN Phosphoramidic acid, [9-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 154534-47-1 HCAPLUS
 CN Phosphoramidic acid, (9-.beta.-D-ribofuranosyl-9H-purin-6-yl)-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



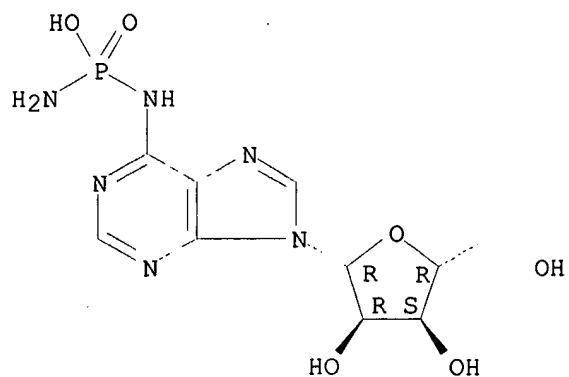
RN 154971-59-2 HCAPLUS
 CN Phosphorodiamidic acid, (9-.beta.-D-ribofuranosyl-9H-purin-6-yl)-, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 154971-58-1
 CMF C10 H15 N6 O6 P
 CDES 5:B-D-RIBO

Searched by: Mary Hale 308-4258 CM-1 1E01

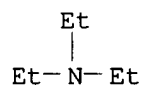
Absolute stereochemistry.



CM 2

CRN 121-44-8

CMF C6 H15 N



RN 154971-64-9 HCAPLUS

CN Phosphoramidic acid, (9-.beta.-D-ribofuranosyl-9H-purin-6-yl)-, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

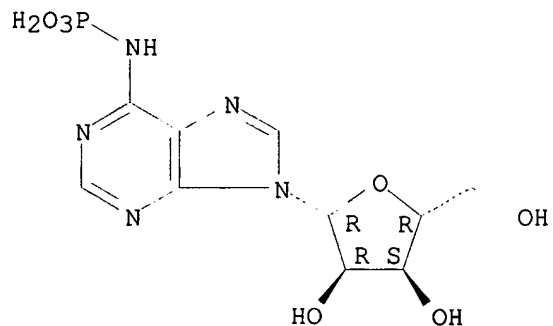
CM 1

CRN 83305-95-7

CMF C10 H14 N5 O7 P

CDES 5:B-D-RIBO

Absolute stereochemistry.

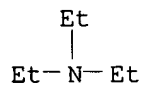


CM 2

CRN 121-44-8

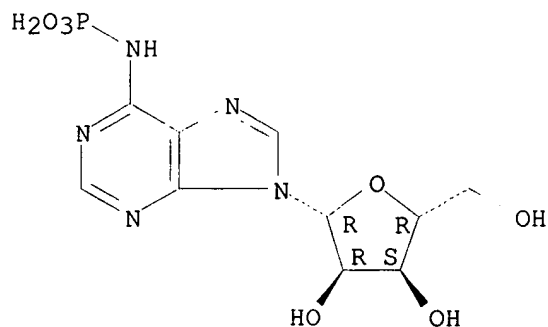
CMF C6 H15 N

Searched by: Mary Hale 308-4258 CM-1 1E01



RN 154971-66-1 HCAPLUS
 CN Phosphoramidic acid, (9-.beta.-D-ribofuranosyl-9H-purin-6-yl)-, disodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.



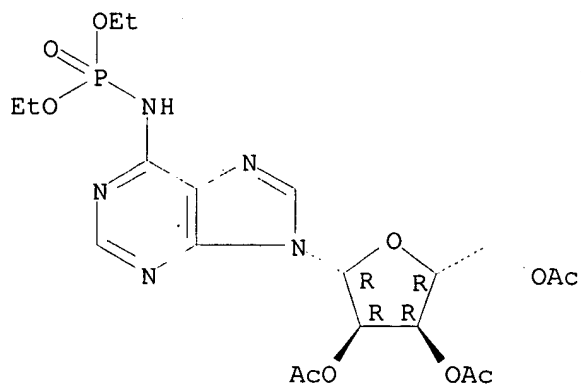
● 2 Na

RN 154971-67-2 HCAPLUS
 CN Phosphoramidic acid, [9-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, diethyl ester, compd. with N,N-diethylethanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

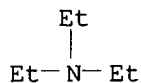
CRN 154534-46-0
 CMF C20 H28 N5 O10 P
 CDES 5:B-D-RIBO

Absolute stereochemistry.



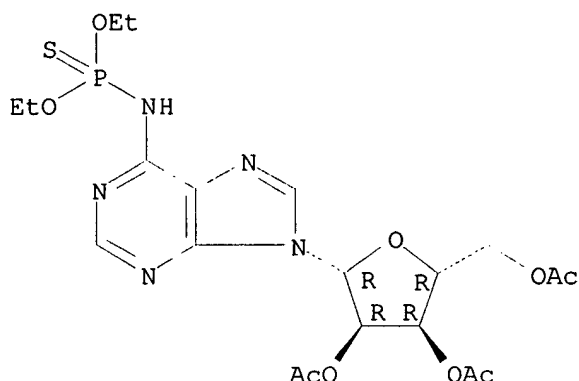
CM 2

CRN 121-44-8
CMF C6 H15 N



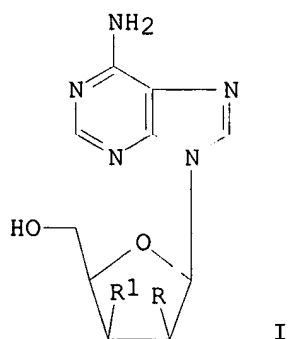
RN 154971-69-4 HCAPLUS
CN Phosphoramidothioic acid, [9-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, O,O-diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 17 OF 77 HCAPLUS COPYRIGHT 2002 ACS
1994:271041 Document No. 120:271041 Nucleic acid related compounds. 81.
Syntheses of 9-(3-deoxy-.beta.-D-threo-pentofuranosyl)adenine, the core nucleoside of the extraordinarily selective antibiotic agrocin 84, and simplified structural component analogs. Vinayak, Ravi; Hansske, Fritz; Robins, Morris J. (Dep. Chem., Univ. Alberta, Edmonton, AB, Can.). J. Heterocycl. Chem., 30(5), 1181-9 (English) 1993. CODEN: JHTCAD. ISSN: 0022-152X.

GI



AB Alternative syntheses of (deoxy-.beta.-D-threo-pentofuranosyl)adenine I (R = OH, R1 = H) (II), the core nucleoside of agrocin 84 and its 2'-deoxy threo isomer I (R = H, R1 = OH) (III) were devised: (1) direct conversion of 9-(.beta.-D-arabinofuranosyl)adenine into 9-(2,3-anhydro-.beta.-D-

Searched by: Mary Hale 308-4258 CM-1 1E01

lyxofuranosyl)adenine and regioselective opening of its oxirane ring with sodium borohydride to give II and III (.apprx.7.5:1); (2) treatment of adenosine with sodium hydride and 2,4,6-triisopropylbenzenesulfonyl chloride, and subjection of the resulting 2'(3')-sulfonates to the reductive [1,2]-hydride shift rearrangement with lithium triethylborohydride to give II and III (.apprx.2:1); and (3) subjection of the phenoxythiocarbonyl esters of 9-[2(3),5-bis-O-(tert-butyldimethylsilyl)-.beta.-D-arabinofuranosyl]adenine to Barton deoxygenation, and deprotection to give II and 2'-deoxyadenosine (.apprx.5:1). Methods (2) and (3) gave lower yields. Syntheses of simplified 6-N- and 5'-O-adenosine phosphoramidate model compds. were explored to examine potential access to such features in the structure proposed for agrocin 84.

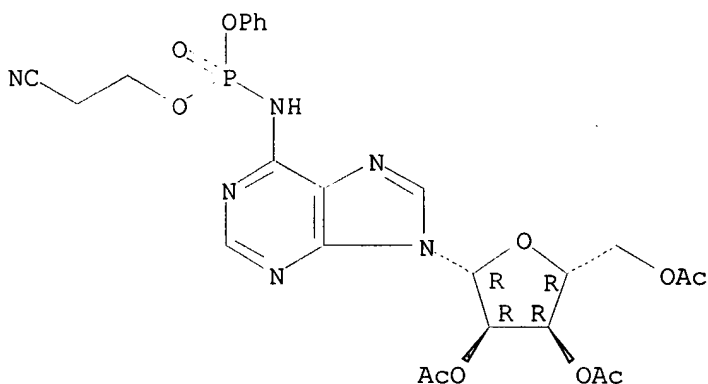
IT 78098-69-8P 154534-35-7P 154534-37-9P
154534-38-0P 154534-39-1P 154534-40-4P
154534-46-0P 154534-48-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and deacetylation of)

RN 78098-69-8 HCAPLUS

CN Phosphoramidic acid, [9-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, 2-cyanoethyl phenyl ester (9CI) (CA INDEX NAME)

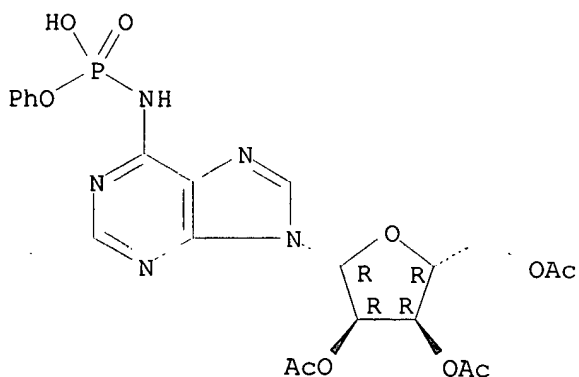
Absolute stereochemistry.



RN 154534-35-7 HCAPLUS

CN Phosphoramidic acid, [9-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, monophenyl ester (9CI) (CA INDEX NAME)

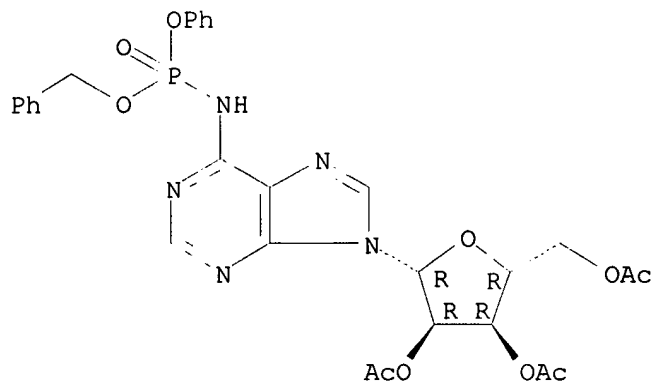
Absolute stereochemistry.



RN 154534-37-9 HCAPLUS

CN Phosphoramidic acid, [9-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, phenyl phenylmethyl ester (9CI) (CA INDEX NAME)

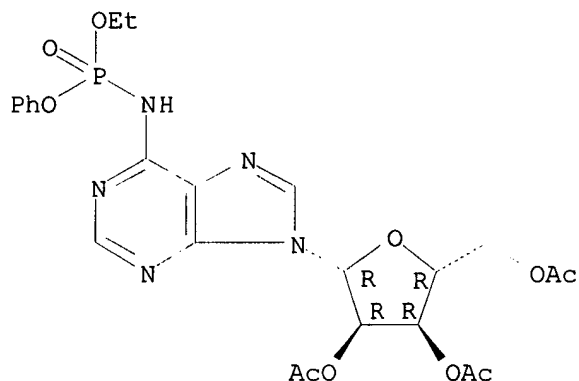
Absolute stereochemistry.



RN 154534-38-0 HCAPLUS

CN Phosphoramidic acid, [9-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, ethyl phenyl ester (9CI) (CA INDEX NAME)

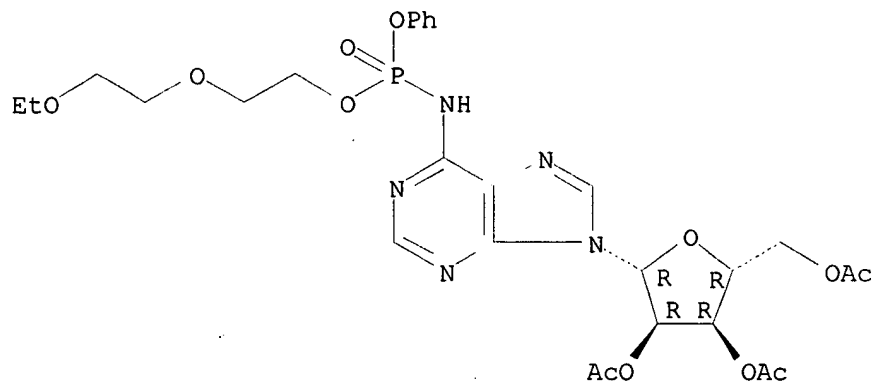
Absolute stereochemistry.



RN 154534-39-1 HCAPLUS

CN Phosphoramidic acid, [9-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, 2-(2-ethoxyethoxy)ethyl phenyl ester (9CI) (CA INDEX NAME)

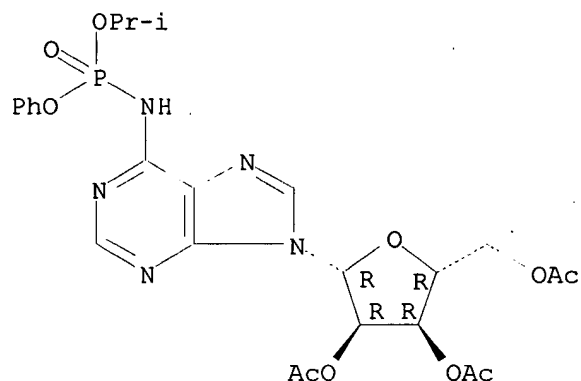
Absolute stereochemistry.



RN 154534-40-4 HCAPLUS

CN Phosphoramidic acid, [9-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, 1-methylethyl phenyl ester (9CI) (CA INDEX NAME)

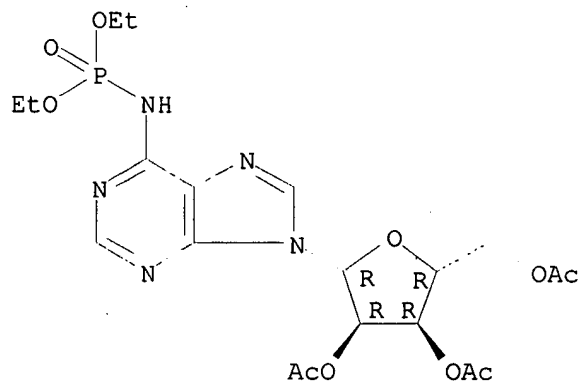
Absolute stereochemistry.



RN 154534-46-0 HCAPLUS

CN Phosphoramidic acid, [9-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

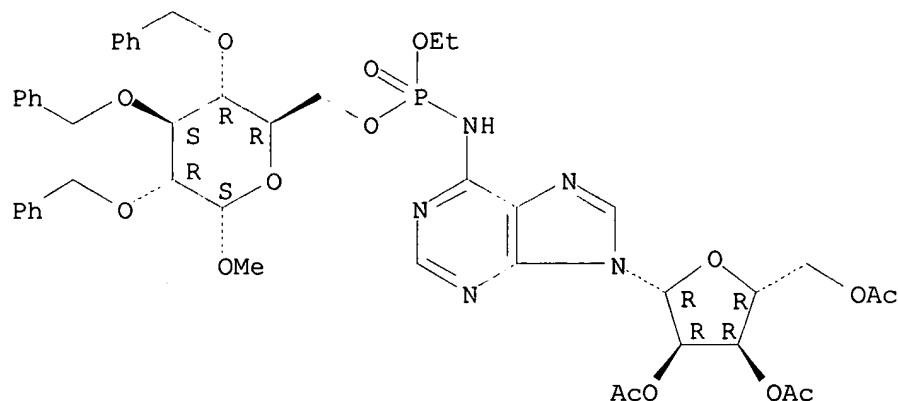


RN 154534-48-2 HCAPLUS

Searched by: Mary Hale 308-4258 CM-1 1E01

CN .alpha.-D-Glucopyranoside, methyl 2,3,4-tris-O-(phenylmethyl)-, ethyl
[9-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)-9H-purin-6-
yl]phosphoramidate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



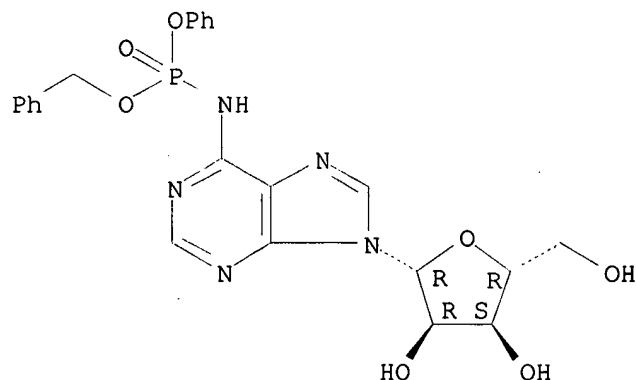
IT 154534-41-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and hydrogenolysis of)

RN 154534-41-5 HCAPLUS

CN Phosphoramidic acid, (9-.beta.-D-ribofuranosyl-9H-purin-6-yl)-, phenyl
phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 78098-64-3P 78111-43-0P 154534-36-8P

154534-42-6P 154534-43-7P 154534-44-8P

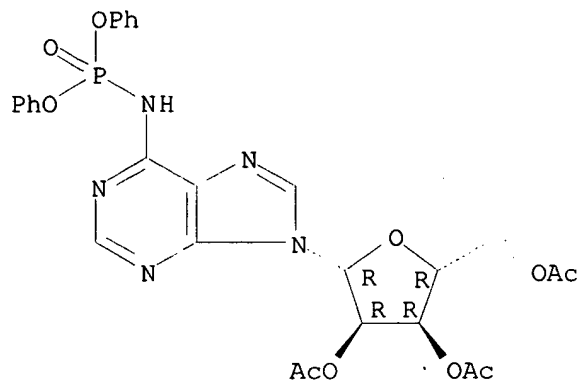
154534-47-1P 154534-49-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 78098-64-3 HCAPLUS

CN Phosphoramidic acid, [9-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)-9H-
purin-6-yl]-, diphenyl ester (9CI) (CA INDEX NAME)

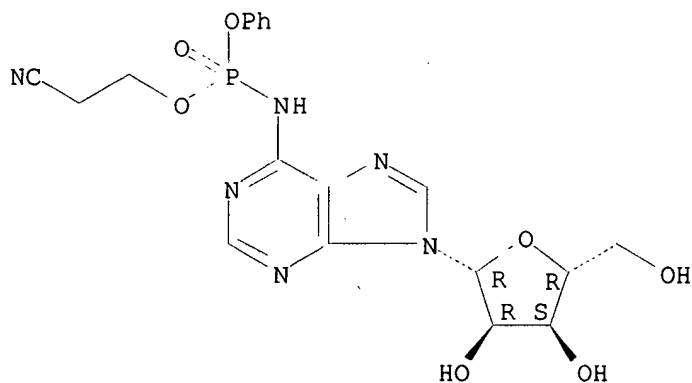
Absolute stereochemistry.



RN 78111-43-0 HCAPLUS

CN Adenosine, N-[(2-cyanoethoxy)phenoxyphosphinyl]- (9CI) (CA INDEX NAME)

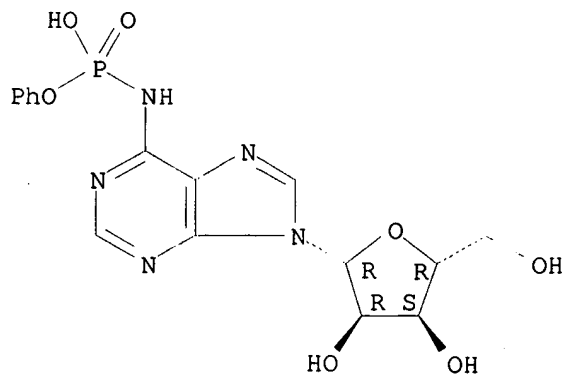
Absolute stereochemistry.



RN 154534-36-8 HCAPLUS

CN Phosphoramidic acid, (9-.beta.-D-ribofuranosyl-9H-purin-6-yl)-, monophenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

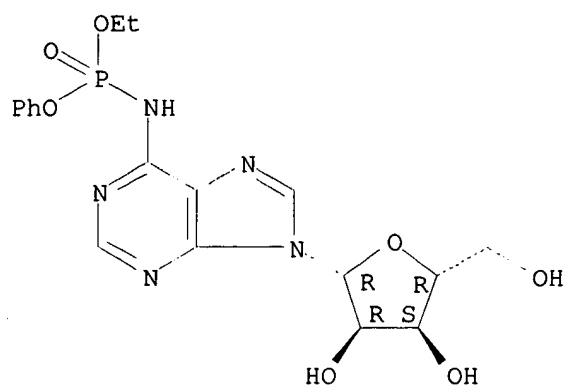


RN 154534-42-6 HCAPLUS

CN Phosphoramidic acid, (9-.beta.-D-ribofuranosyl-9H-purin-6-yl)-, ethyl phenyl ester (9CI) (CA INDEX NAME)

Searched by: Mary Hale 308-4258 CM-1 1E01

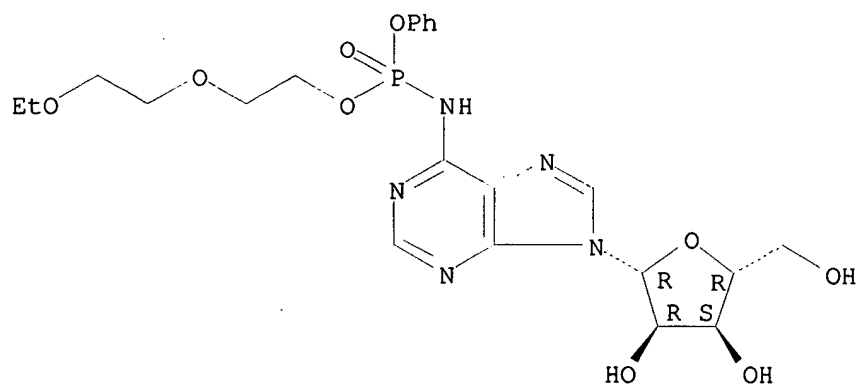
Absolute stereochemistry.



RN 154534-43-7 HCAPLUS

CN Phosphoramidic acid, (9-.beta.-D-ribofuranosyl-9H-purin-6-yl)-, 2-(2-ethoxyethoxy)ethyl phenyl ester (9CI) (CA INDEX NAME)

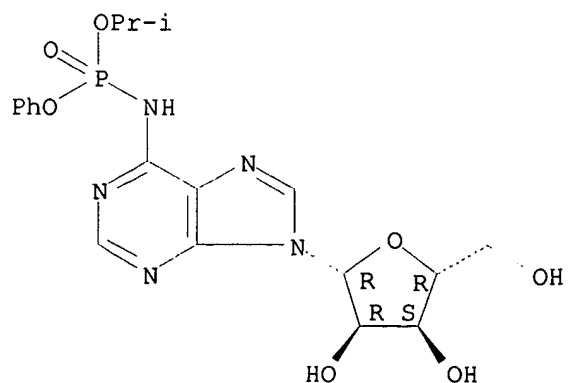
Absolute stereochemistry.



RN 154534-44-8 HCAPLUS

CN Phosphoramidic acid, (9-.beta.-D-ribofuranosyl-9H-purin-6-yl)-, 1-methylethyl phenyl ester (9CI) (CA INDEX NAME)

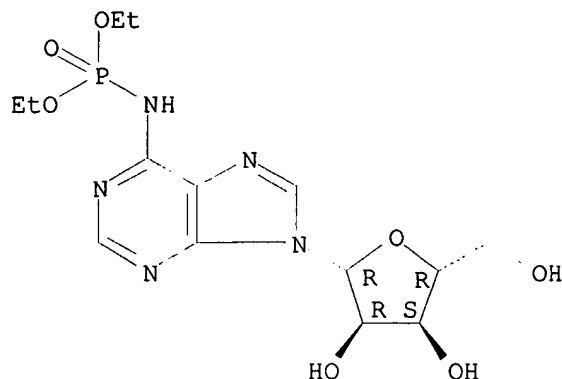
Absolute stereochemistry.



Searched by: Mary Hale 308-4258 CM-1 1E01

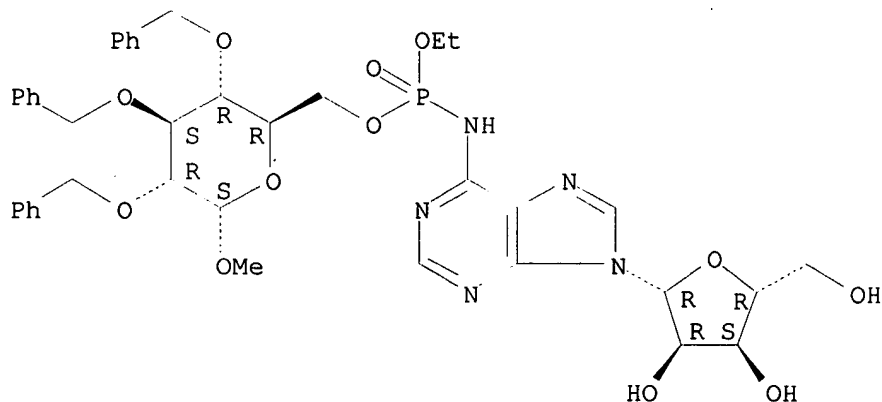
RN 154534-47-1 HCAPLUS
 CN Phosphoramidic acid, (9-.beta.-D-ribofuranosyl-9H-purin-6-yl)-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



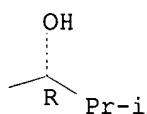
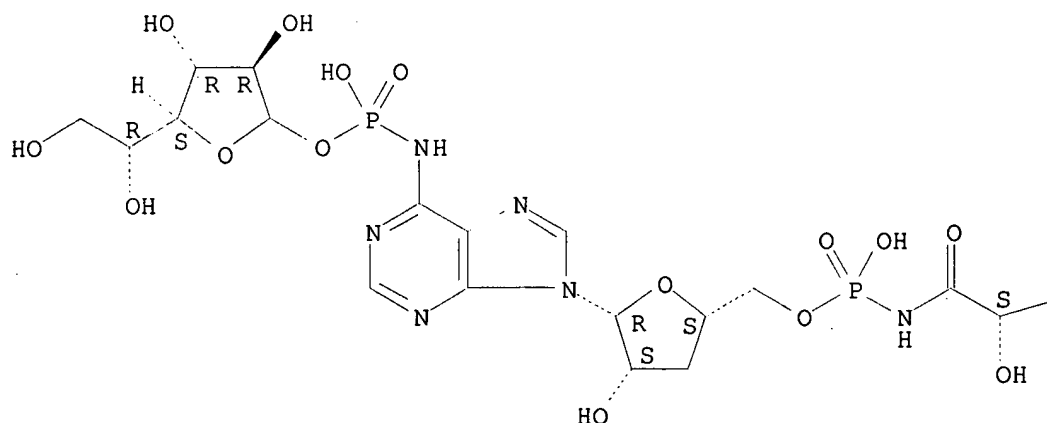
RN 154534-49-3 HCAPLUS
 CN .alpha.-D-Glucopyranoside, methyl 2,3,4-tris-O-(phenylmethyl)-, ethyl (9-.beta.-D-ribofuranosyl-9H-purin-6-yl)phosphoramidate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **59111-78-3P**, Agrocin 84
 RL: SPN (Synthetic preparation); PREP (Preparation)
 . (prepn. of (deoxythreopentofuranosyl)adenine segment of)
 RN 59111-78-3 HCAPLUS
 CN D-Glucofuranose, 1-[hydrogen [9-[3-deoxy-5-O-[[(4,5-dideoxy-4-methyl-D-threo-pentonoyl)amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 18 OF 77 HCAPLUS COPYRIGHT 2002 ACS

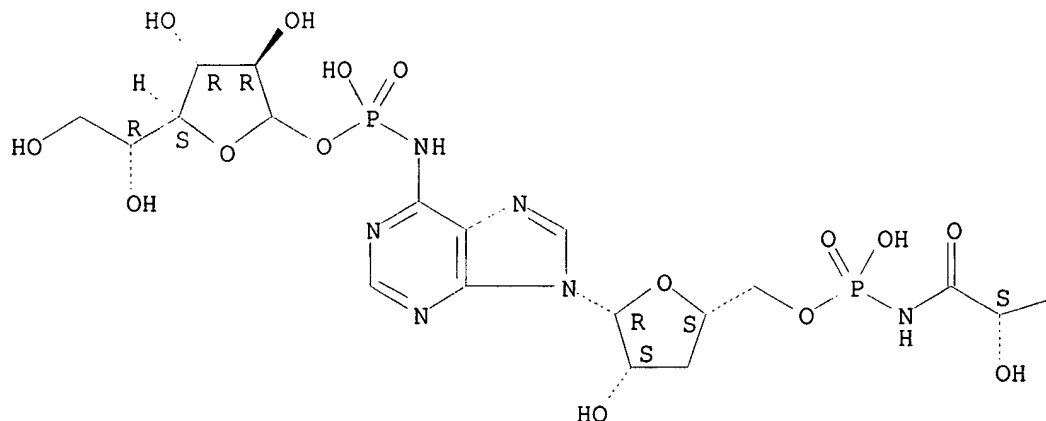
1994:24582 Document No. 120:24582 Genetic analysis of the agrocinopine catabolic region of *Agrobacterium tumefaciens* Ti plasmid pTiC58, which encodes genes required for opine and agrocin 84 transport. Hayman, G. Thomas; Beck von Bodman, Susanne; Kim, Heenam; Jiang, Ping; Farrand, Stephen K. (Med. Cent., Loyola Univ., Maywood, IL, 60153, USA). *J. Bacteriol.*, 175(17), 5575-84 (English) 1993. CODEN: JOBAAY. ISSN: 0021-9193.

AB The acc region, subcloned from pTiC58 of classical nopaline and agrocinopine A and B *Agrobacterium tumefaciens* C58, allowed agrobacteria to grow using agrocinopine B as the sole source of carbon and energy. Acc is .apprx.6 kb in size. It consists of .gtoreq.5 genes, accA through accE, as defined by complementation anal. using subcloned fragments and transposon insertion mutations of acc carried on different plasmids within the same cells. All 5 regions are required for agrocin 84 sensitivity, and .gtoreq.4 are required for agrocinopine and agrocin 84 uptake. The complementation results are consistent with the hypothesis that each of the 5 regions is sep. transcribed. Maxicell expts. showed that the first of these genes, accA, encodes a 60-kDa protein. Anal. of osmotic shock fractions showed this protein to be located in the periplasm. The DNA sequence of the accA region revealed an open reading frame encoding a predicted polypeptide of 59,147 Da. The amino acid sequence encoded by this open reading frame is similar to the periplasmic binding proteins OppA and Dppa of *Escherichia coli* and *Salmonella typhimurium* and OppA of

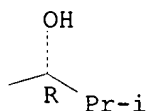
Bacillus subtilis.
 IT 59111-78-3, Agrocine 84
 RL: PRP (Properties)
 (susceptibility to, genes acc for, of Agrobacterium tumefaciens plasmid pTiC58)
 RN 59111-78-3 HCAPLUS
 CN D-Glucosyl, 1-[hydrogen [9-[3-deoxy-5-O-[[4,5-dideoxy-4-methyl-D-threo-pentonyl]amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



L7 ANSWER 19 OF 77 HCAPLUS COPYRIGHT 2002 ACS
 1994:24551 Document No. 120:24551 Functional and mutated agrocineopine synthase genes on octopine T-DNAs. Paulus, Francois; Otten, Leon (Plant Mol. Biol. Lab., CNRS, Strasbourg, 67084, Fr.). Mol. Plant-Microbe Interact., 6(3), 393-402 (English) 1993. CODEN: MPMIEL. ISSN: 0894-0282.
 AB Agrocineopine synthase genes have so far been detected only on the Agrobacterium tumefaciens nopaline Ti plasmid pTiC58 and on the A. rhizogenes Ri plasmid pRiA4. The TA region of the octopine/cucumopine (o/c) A. vitis Ti plasmid pTiTm4 strongly resembles the TL DNA of biotype I octopine Ti plasmids. In addn., it carries an intact and functional agrocineopine synthase gene close to its left border. TA/TL sequence comparison shows that the biotype I TL region still carries a 5'-deleted acs gene, strongly indicating that this gene was originally part of the TL

Searched by: Mary Hale 308-4258 CM-1 1E01

region and belongs to the "common DNA" region of octopine and nopaline Ti plasmids. Tm4 and C58C1 (pTiTm4) remove agrocinopine A from the medium indicating that pTiTm4 also carries agrocinopine uptake genes. In spite of this, Tm4 and related strains are resistant against agrocin 84. Two o/c Ti plasmids that are closely related to pTiTm4, pTiHm1, and pTiAB3, have a mutated acs gene; whereas Hm1 can still take up agrocinopine A, AB3 cannot. These results yield new insights in the evolution of octopine, nopaline, and o/c strains.

IT 59111-78-3, Agrocin 84

RL: PRP (Properties)

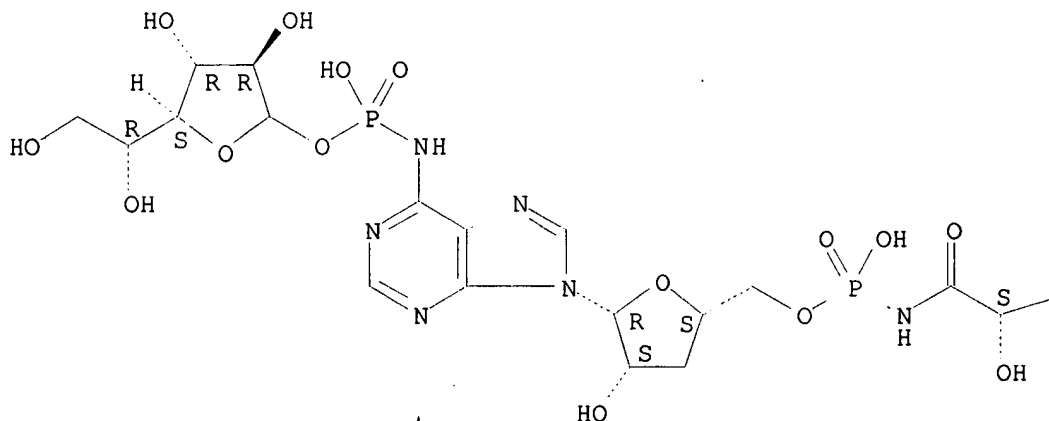
(resistance to, Ti plasmids of *Agrobacterium tumefaciens* conferring, agrocinopine synthase genes and agrocinopine uptake in relation to)

RN 59111-78-3 HCAPLUS

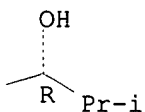
CN D-Glucofuranose, 1-[hydrogen [9-[3-deoxy-5-O-[[[(4,5-dideoxy-4-methyl-D-threo-pentono-yl)amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



L7 ANSWER 20 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1993:449805 Document No. 119:49805 Synthesis and properties of adenosine 6-N-phosphoramidate. Wada, Takeshi; Moriguchi, Tomohisa; Sekine, Mitsuo (Fac. Biosci. Biotechnol., Tokyo Inst. Technol., Tokohama, 227, Japan). Nucleic Acids Symp. Ser., 27(Nineteenth Symposium on Nucleic Acids Chemistry, 1992), 93-4 (English) 1992. CODEN: NACSD8. ISSN: 0261-3166.

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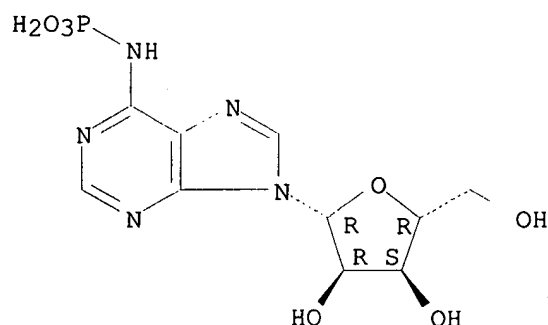
AB A symposium report of a new class of phosphorlyated nucleosides, e.g. adenosine 6-N-phosphoramidate (6-N-AMP) and its derivs. which were synthesized and their properties investigated.

IT **83305-95-7P**
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn. and properties of)

RN 83305-95-7 HCAPLUS

CN Phosphoramidic acid, (9-.beta.-D-ribofuranosyl-9H-purin-6-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 21 OF 77 HCAPLUS COPYRIGHT 2002 ACS
 1993:404989 Document No. 119:4989 Zeatin allylic phosphate: occurrence, formation and possible role. Vonk, C. R.; Davelaar, E. (Cent. Agrobiol. Res., Wageningen, 6700 AA, Neth.). Curr. Plant Sci. Biotechnol. Agric., 13(Prog. Plant Growth Regul.), 617-23 (English) 1992. CODEN: CPBAE2. ISSN: 0924-1949.

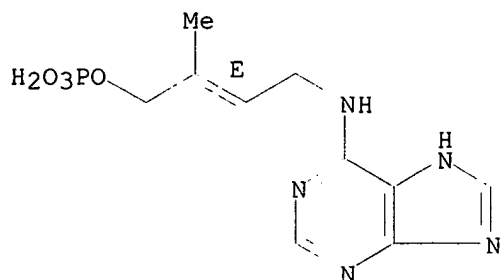
AB Formation of zeatin allylic phosphate (ZAP) by a biol. system has been demonstrated by incubation of a microsomal fraction prepd. from bulb disks of iris and also by a microsomal fraction prepd. in the same way from Helianthus tubers. Treatment of the microsomal fraction with Triton X-100 resulted in a sol. fraction showing ZAP-forming activity. This fraction was partially purified by Ultrogel HA-column chromatog. Ultrafree-MC filter units were used to further purify the ZAP-forming fraction, resulting in a five-fold increase in specific activity. Enzyme activity was optimal at a concn. of 4 .mu.g/mL of added partially purified microsomal protein and decreased at higher protein concn. The enzyme activity of Triton X-100 solubilized microsomal membranes was inhibited by pronase digestion (68% inhibition), and was completely destroyed in the presence of 0.5% SDS (final vol.) or after heat treatment (10 min, 100.degree.). The greatest quantity of ZAP-forming enzyme activity was present in the intracellular membrane fraction. This enzyme specifically recognizes the trans-form of zeatin rather than cis-zeatin or dihydrozeatin.

IT **124031-41-0**
 RL: BIOL (Biological study)
 (formation and role of, in Helianthus tuberosus, enzyme in)

RN 124031-41-0 HCAPLUS

CN 2-Buten-1-ol, 2-methyl-4-(1H-purin-6-ylamino)-, dihydrogen phosphate (ester), (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L7 ANSWER 22 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1993:97956 Document No. 118:97956 Biological control of *Agrobacterium tumefaciens*, colonization, and pAgK84 transfer with *Agrobacterium radiobacter* K84 and the Tra- mutant strain K1026. Vicedo, Begonya; Penalver, Ramon; Asins, Maria Jose; Lopez, Maria M. (Inst. Valenciano Invest. Agrarias, Valencia, 46113, Spain). Appl. Environ. Microbiol., 59(1), 309-15 (English) 1993. CODEN: AEMIDF. ISSN: 0099-2240.

AB The efficacies of *A. radiobacter* K84 and K1026 in root colonization, crown gall control, and plasmid transfer were compared. Levels of root colonization by K84 and K1026 of Montclar and Nemaguard peach seedlings were similar during the 21 days of the expt. Four strains of *A. tumefaciens* bv. 1 were used for soil inoculations in biol. control expts. on GF677 and Adafuel peach .times. almond rootstocks; 2 were sensitive and 2 were resistant to agrocin 84. Both strains K84 and K1026 were very efficient in controlling the sensitive strains, but some tumors appeared with both treatments. In the biocontrol of resistant strains, no galls were obsd. in K1026-treated plants, but some K84-treated plants had galls. Recovery of agrobacteria from galls in expts. with sensitive and resistant strains showed that all of the isolates from the controls or K1026-treated plants and most of the isolates from K84-treated plants had the same characteristics as the inoculated strains. Nine isolates from the K84-treated plants growing in soil inoculated with 1 resistant strain were virulent and produced agrocin 84. These isolates had a plasmid that hybridized with a probe prepd. with the BamHI C fragment from pAgK84. These results show the efficiency of K1026 in biocontrol of agrocin 84-sensitive and -resistant strains of *A. tumefaciens* and suggest the use of K1026 as a safer organism than K84 for biol. control of crown gall.

IT 59111-78-3, Agrocin 84

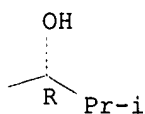
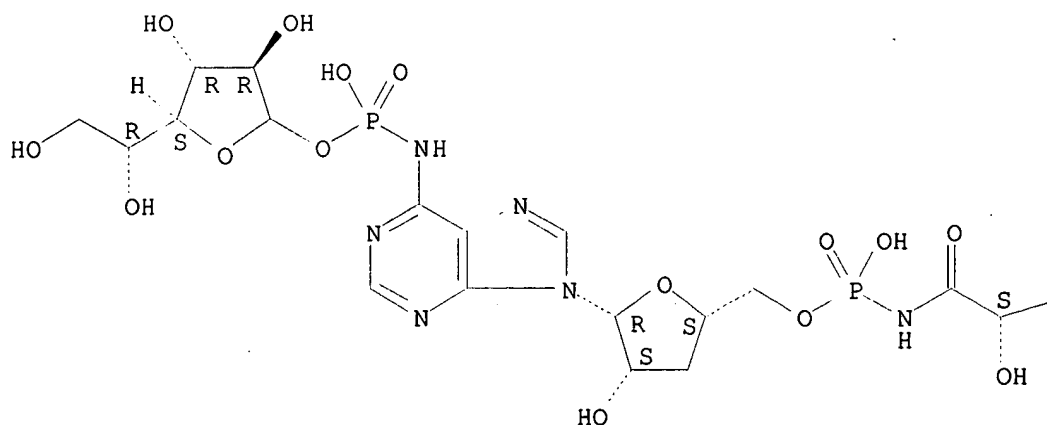
RL: BIOL (Biological study)

(*Agrobacterium tumefaciens* sensitive and resistant to, biol. control of)

RN 59111-78-3 HCAPLUS

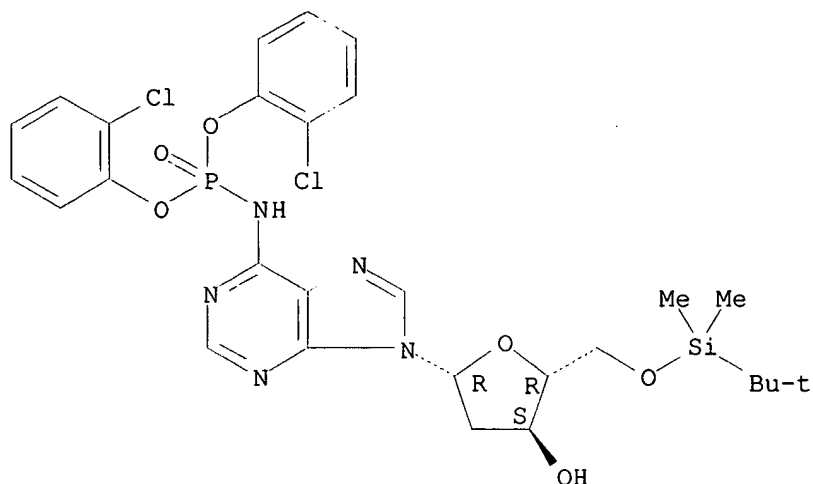
CN D-Glucufuranose, 1-[hydrogen [9-[3-deoxy-5-O-[[[4,5-dideoxy-4-methyl-D-threo-pentonoyl)amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



- L7 ANSWER 23 OF 77 HCAPLUS COPYRIGHT 2002 ACS
 1993:81317 Document No. 118:81317 O-selective phosphorylation of nucleosides without N-protection. Uchiyama, Mamoru; Aso, Yoshio; Noyori, Ryoji; Hayakawa, Yoshihiro (Fac. Sci., Nagoya Univ., Nagoya, 464-01, Japan). J. Org. Chem., 58(2), 373-9 (English) 1993. CODEN: JOCEAH. ISSN: 0022-3263. OTHER SOURCES: CASREACT 118:81317.
- AB A facile chemoselective O-phosphorylation of N-unprotected nucleosides has been achieved via metal alkoxide formation. Sequential treatment of N-unprotected nucleosides with an equimolar amt. of an organometallic base, such as an alkyllithium, Me₃COK, Me₃CMgCl, LiAl(NMe₂)₄, Al(NMe₂)₃, (Me₂CHCH₂)₂AlH, etc., and a phosphorochloridate or p-nitrophenyl phosphate results in rapid O-phosphorylation to give the nucleotides in high yield. The method using magnesium alkoxides is the best in chemoselectivity, generality, and operational simplicity. The origin of the obsd. chemoselectivity is discussed.
- IT **145550-40-9P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
- RN 145550-40-9 HCAPLUS
 CN Phosphoramidic acid, [[2-deoxy-5-O-[(1,1-dimethylethyl)dimethylsilyl]-.beta.-D-erythro-pentofuranosyl]-9H-purin-6-yl]-, bis(2-chlorophenyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



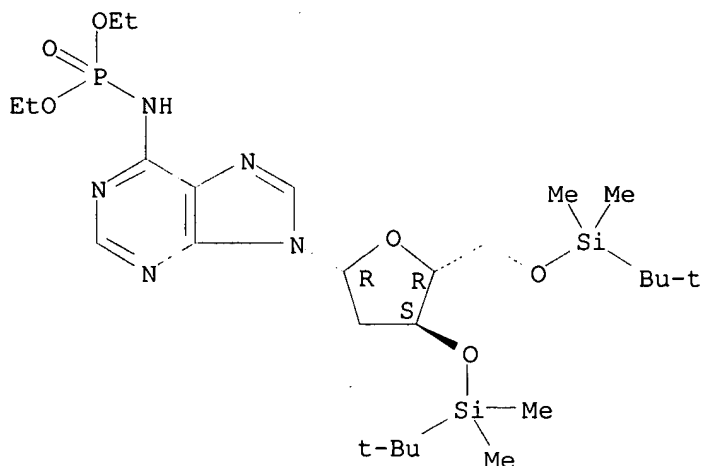
IT 145550-43-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(regioselective prepn. of, from unprotected nucleoside)

RN 145550-43-2 HCAPLUS

CN Phosphoramidic acid, [[2-deoxy-3,5-bis-O-[(1,1-dimethylethyl)dimethylsilyl]-.beta.-D-erythro-pentofuranosyl]-9H-purin-6-yl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 24 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1991:626021 Document No. 115:226021 Biological control of crown gall with Agrobacterium radiobacter strain K84. Yokoyama, Tomoko (Chiba Prefect. Agric. Exp. Stn., Chiba, 280-02, Japan). Shokubutsu Boeki, 45(8), 337-40 (Japanese) 1991. CODEN: SHBOAO. ISSN: 0037-4091.

AB A review with 11 refs. on the modes of action of A. radiobacter K 84 and AArocin 84 produced by this strain against crown gall, deactivation of the strain by the fusion with the pathogen, construction of a new Agrocin 84-producing strain K 1026 by gene technol., and their application.

IT 59111-78-3, Agrocin 84

RL: BIOL (Biological study)
(crown gall control with)

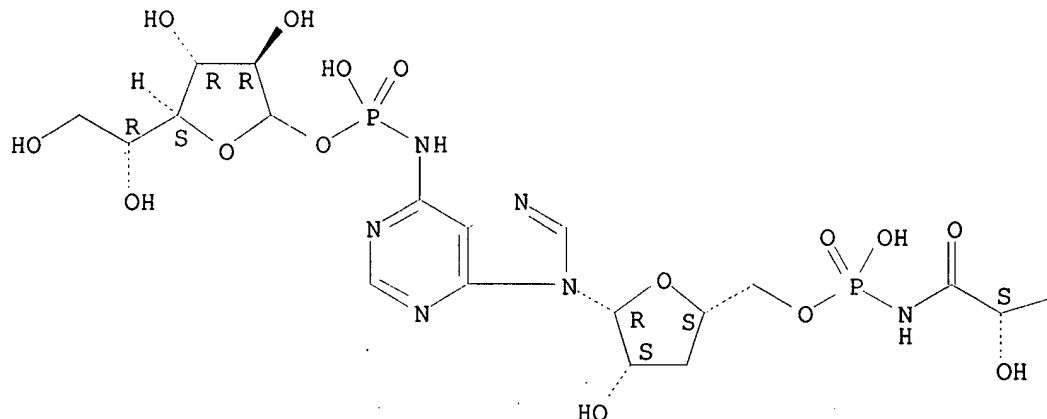
Searched by: Mary Hale 308-4258 CM-1 1E01

RN 59111-78-3 HCAPLUS

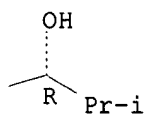
CN D-Glucofuranose, 1-[hydrogen [9-[3-deoxy-5-O-[[[4,5-dideoxy-4-methyl-D-threo-pentonoyl)amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



L7 ANSWER 25 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1991:1281 Document No. 114:1281 Agrobacterium plasmids encode structurally and functionally different loci for catabolism of agrocinopine-type opines. Hayman, G. Thomas; Farrand, Stephen K. (Med. Cent., Loyola Univ., Maywood, IL, 60153, USA). Mol. Gen. Genet., 223(3), 465-73 (English) 1990. CODEN: MGGEAE. ISSN: 0026-8925.

AB Agrobacterium tumefaciens strains C58, T37, K827 and J73, A. rhizogenes strains A4 and 15834, and A. radiobacter strain K299 were all susceptible to agrocin 84 and this sensitivity was enhanced in each case by addn. of agrocinopines A and B. Anal. of transconjugants showed that sensitivity of strain A4 to agrocin 84 was encoded by pArA4a and not by the rhizogenic plasmid, pRiA4. The acc region of the A. tumefaciens nopaline-type Ti plasmid pTiC58, contained on the recombinant plasmid pTHH206, hybridized strongly to restriction fragments of plasmids from strains T37, K827, J73 and K299. Hybridizing fragment patterns generated with BamHI and EcoRI were identical among the 4 Ti plasmids while pAtK299 showed restriction fragment length polymorphisms at acc with the 2 enzymes. At moderate stringency, the pTiC58 acc region hybridized weakly to a single

Searched by: Mary Hale 308-4258 CM-1 1E01

restriction fragment from the Ar plasmid of *A. rhizogenes* strain A4, but not to pTiBo542, which encodes catabolism of the closely related opines agrocinopines C and D. Plasmid pAtK84b of *A. radiobacter* strain K84 is induced for conjugal transfer by agrocinopines A and B. However, no hybridization was detected between this plasmid and acc from pTiC58 under conditions of moderate stringency. Like pTiC58, pAtK84b conferred transport of agrocinopines A and B on its host bacteria despite the absence of detectable sequence homol. with the pTiC58-derived acc probe. However, unlike pTiC58, pAtK84b failed to confer sensitivity to or uptake of agrocin 84 on its bacterial host. These results indicate that at least 4 distinguishable systems exist for catabolism of the 2 agrocinopine opine families with the prototype locus, exemplified by acc from pTiC58, being strongly conserved among nopaline-type Ti plasmids.

IT 59111-78-3, Agrocin 84

RL: PRP (Properties)

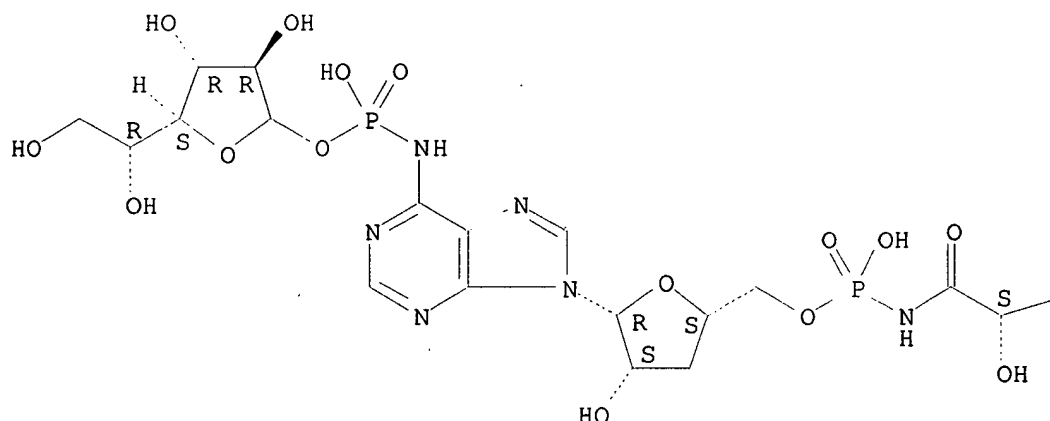
(Agrobacterium susceptibility to, agrocinopines enhancement of, resident plasmid genes in relation to)

RN 59111-78-3 HCAPLUS

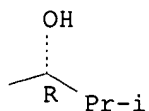
CN D-Glucofuranose, 1-[hydrogen [9-[3-deoxy-5-O-[[[(4,5-dideoxy-4-methyl-D-threo-pentonoyl)amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

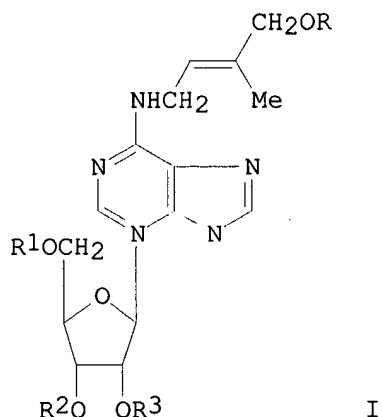


L7 ANSWER 26 OF 77 HCAPLUS COPYRIGHT 2002 ACS

Searched by: Mary Hale 308-4258 CM-1 1E01

1990:572616 Document No. 113:172616 The synthesis of phosphorus derivatives of ribosyl zeatin. Shadid, Belal; Van der Plas, Henk C. (Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.). Tetrahedron, 46(6), 2179-86 (English) 1990. CODEN: TETRAB. ISSN: 0040-4020. OTHER SOURCES: CASREACT 113:172616.

GI



AB Sulfur was used for the conversion of ribosyl zeatin phosphonate I [R = PH(O)OH, R1 = SiMe2CMe3, PH(O)OH, R2R3 = CHOMe] (II) into the corresponding thiophosphates I [R = P(S)(OH)2]. 2,2'-Dipyridyldisulfide in the presence of MeOH was used for the conversion of II into the corresponding Me phosphates I [R = P(O)(OH)OMe]. Deprotection of these compds. gave the phosphorus derivs. of ribosyl zeatin I [R, R1 = H, PH(O)OH, P(O)(OH)OMe, P(S)(OH)2; R2 = R3 = H].

IT **128184-97-4**

RL: PROC (Process)

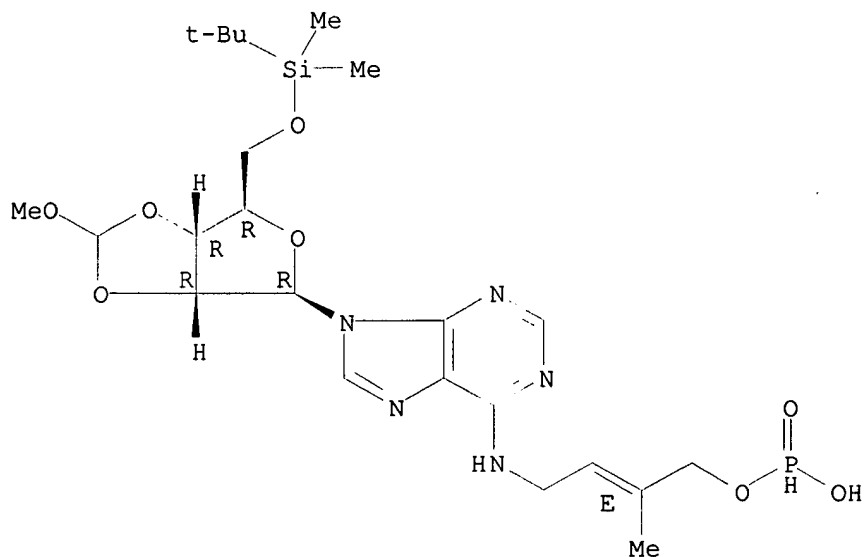
(conversion of, to Me phosphates)

RN 128184-97-4 HCAPLUS

CN Adenosine, 5'-O-[(1,1-dimethylethyl)dimethylsilyl]-N-[4-[(hydroxyphosphinyl)oxy]-3-methyl-2-butenyl]-2',3'-O-(methoxymethylene)-, (E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



IT 129788-91-6P 129788-92-7P 129788-93-8P

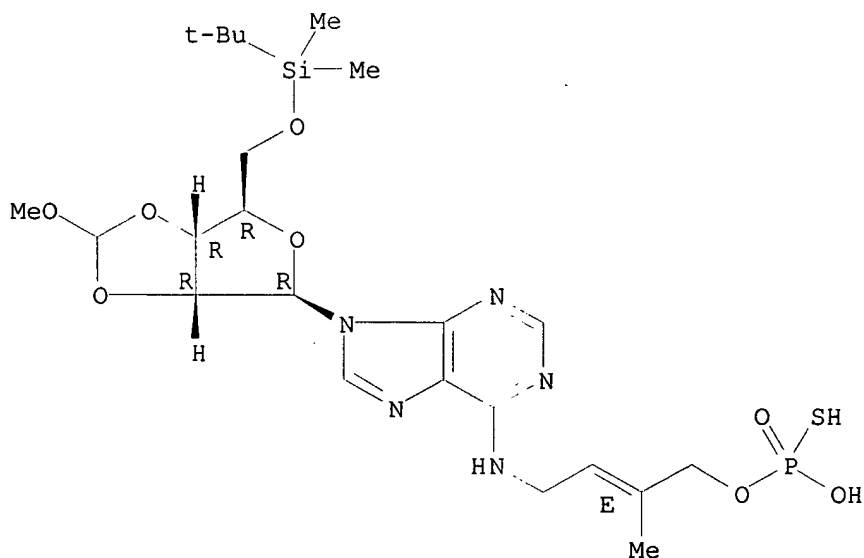
129788-94-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and demethoxymethylidenation of)

RN 129788-91-6 HCAPLUS

CN Adenosine, N-[4-[(hydroxymethoxyphosphinyl)oxy]-3-methyl-2-butenyl]-5'-O-
[(1,1-dimethylethyl)dimethylsilyl]-2',3'-O-(methoxymethylene)-, (E)- (9CI)
(CA INDEX NAME)

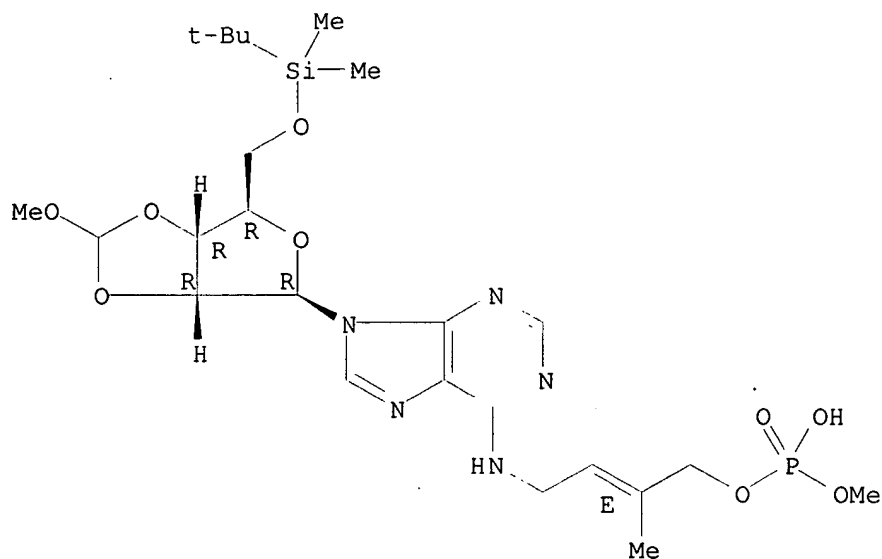
Absolute stereochemistry.
Double bond geometry as shown.



RN 129788-92-7 HCAPLUS

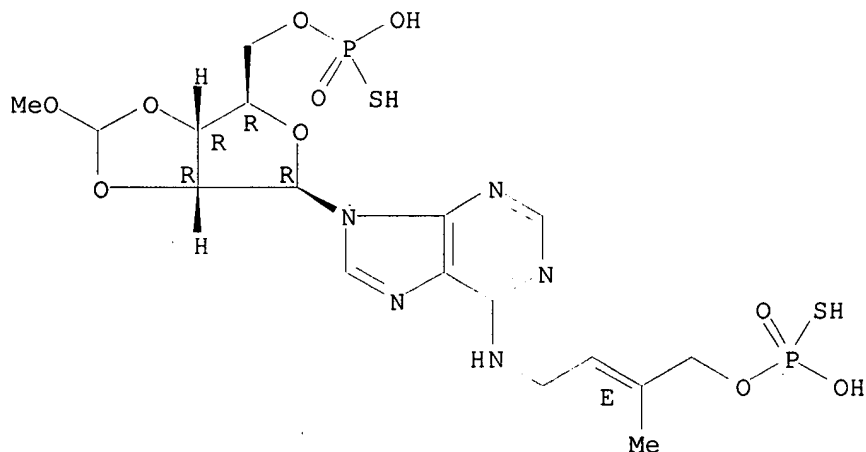
CN Adenosine, 5'-O-[(1,1-dimethylethyl)dimethylsilyl]-N-[4-
[(hydroxymethoxyphosphinyl)oxy]-3-methyl-2-butenyl]-2',3'-O-
(methoxymethylene)-, (E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



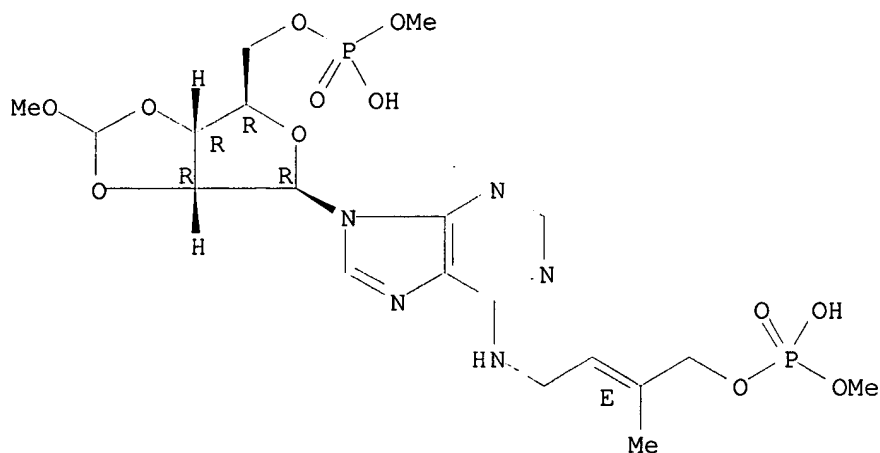
RN 129788-93-8 HCAPLUS
CN Adenosine, N-[4-[(hydroxymercaptophosphinyl)oxy]-3-methyl-2-butenyl]-2',3'-
O-(methoxymethylene)-, 5'-(dihydrogen phosphorothioate), (E)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 129788-94-9 HCAPLUS
CN 5'-Adenylic acid, N-[4-[(hydroxymethoxyphosphinyl)oxy]-3-methyl-2-butenyl]-
2',3'-O-(methoxymethylene)-, 5'-methyl ester, (E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



IT 129788-95-0P 129788-96-1P 129788-97-2P

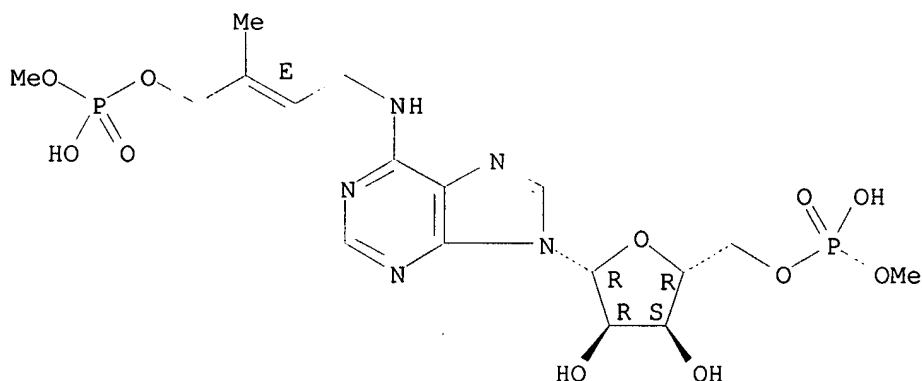
129788-98-3P 129788-99-4P 129789-00-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 129788-95-0 HCAPLUS

CN 5'-Adenylic acid, N-[4-[(hydroxymethoxyphosphinyl)oxy]-3-methyl-2-butenyl]-
, 5'-methyl ester, (E)- (9CI) (CA INDEX NAME)

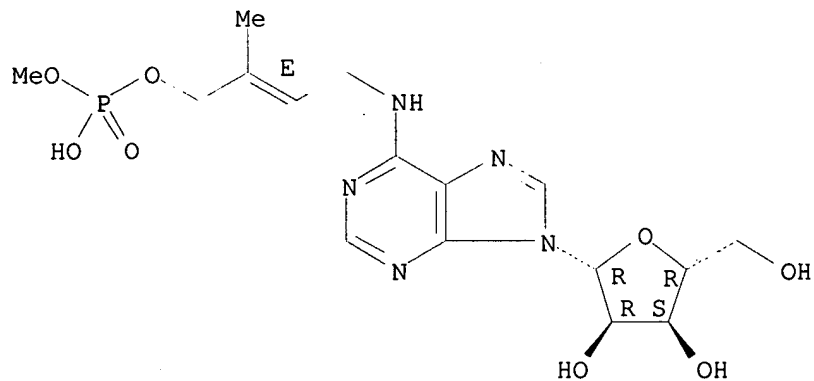
Absolute stereochemistry.
Double bond geometry as shown.



RN 129788-96-1 HCAPLUS

CN Adenosine, N-[4-[(hydroxymethoxyphosphinyl)oxy]-3-methyl-2-butenyl]-, (E)-
(9CI) (CA INDEX NAME)

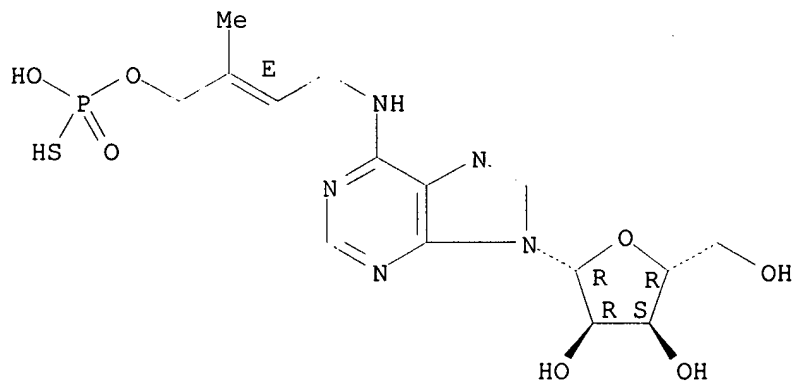
Absolute stereochemistry.
Double bond geometry as shown.



RN 129788-97-2 HCAPLUS

CN Adenosine, N-[4-[(hydroxymethylphosphoryl)oxy]-3-methyl-2-butenyl]-, (E)- (9CI) (CA INDEX NAME)

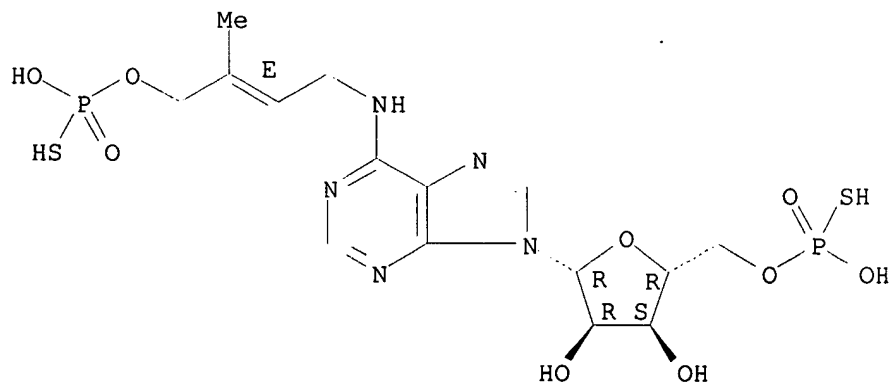
Absolute stereochemistry.
Double bond geometry as shown.



RN 129788-98-3 HCAPLUS

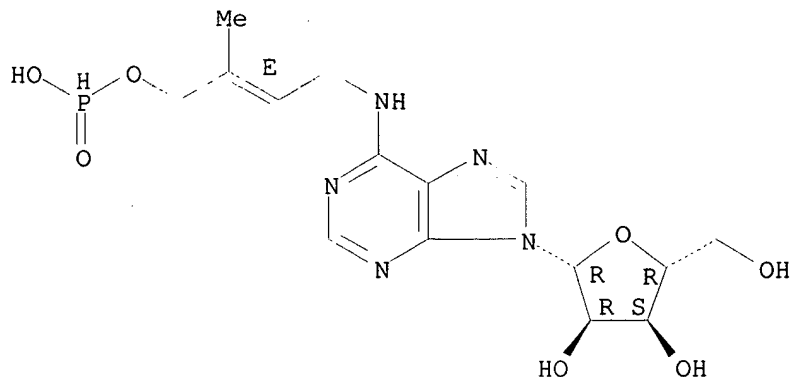
CN Adenosine, N-[4-[(hydroxymethylthio)oxy]-3-methyl-2-butenyl]-, 5'-(dihydrogen phosphorothioate), (E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



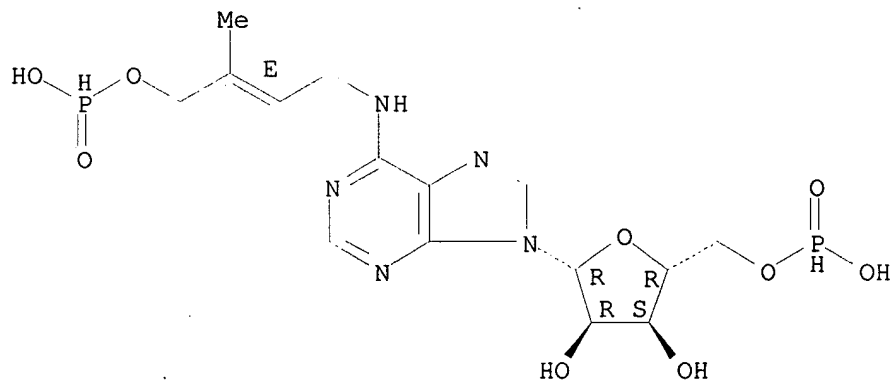
RN 129788-99-4 HCAPLUS
CN Adenosine, N-[4-[(hydroxyphosphinyl)oxy]-3-methyl-2-butenyl]-, (E)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



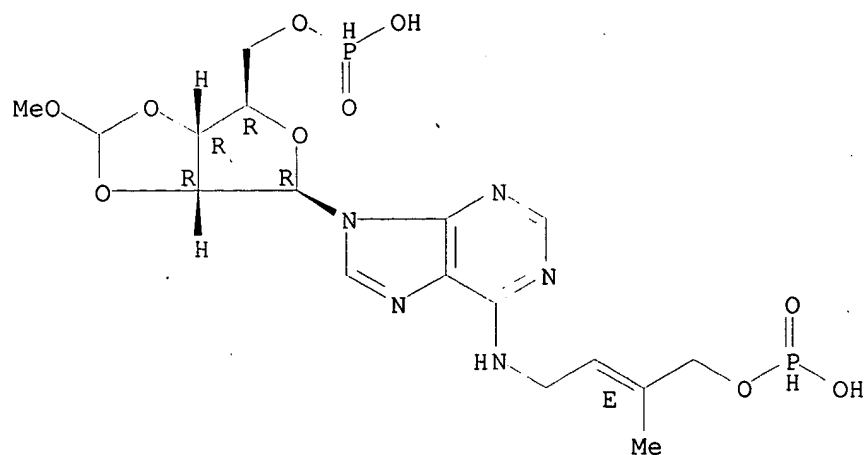
RN 129789-00-0 HCAPLUS
CN Adenosine, N-[4-[(hydroxyphosphinyl)oxy]-3-methyl-2-butenyl]-,
5'-(hydrogen phosphonate), (E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



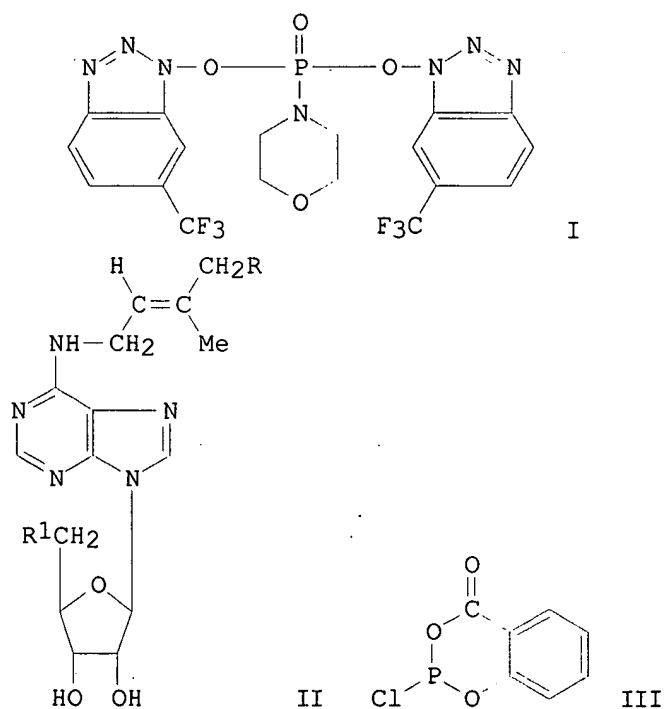
IT 128184-98-5
RL: RCT (Reactant)
(sulfuration of, with sulfur, thiophosphates from)
RN 128184-98-5 HCAPLUS
CN Adenosine, N-[4-[(hydroxyphosphinyl)oxy]-3-methyl-2-butenyl]-2',3'-O-
(methoxymethylene)-, 5'-(hydrogen phosphonate), (E)- (9CI) (CA INDEX
NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L7 ANSWER 27 OF 77 HCAPLUS COPYRIGHT 2002 ACS
 1990:459752 Document No. 113:59752 The synthesis of cytokinin phosphates.
 Shadid, Belal; Van der Plas, Henk C. (Lab. Org. Chem., Agric. Univ.
 Wageningen, Wageningen, 6703 HB, Neth.). Tetrahedron, 46(3), 901-12
 (English) 1990. CODEN: TETRAB. ISSN: 0040-4020. OTHER SOURCES: CASREACT
 113:59752.

GI



AB The bifunctional phosphorylating reagent N-morpholino O,O-bis[6-trifluoromethyl)benzotriazolyl]phosphate I was used for the prepn. of adenosine phosphates II (R = OH, OPO3H2, R1 = OPO3H2), whereas the

monofunctional phosphitylating reagent 2-chlorobenzodioxaphosphorin-3-one III was used for the prepn. of ribosyl zeatin allylic phosphate II (R = OPO₃H₂, R₁ = H) and ribosyl zeatin diphosphate II (R = R₁ = OPO₃H₂).

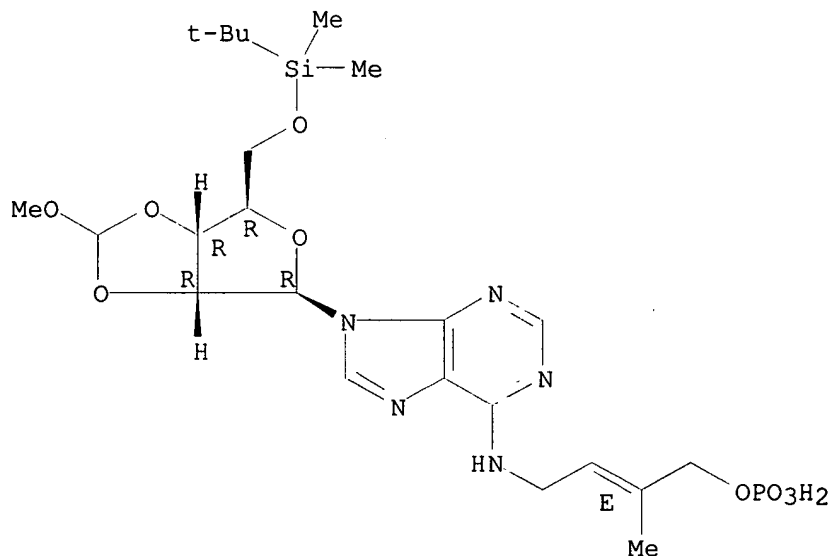
IT 128184-99-6P 128198-65-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and deprotection of)

RN 128184-99-6 HCAPLUS

CN Adenosine, 5'-O-[(1,1-dimethylethyl)dimethylsilyl]-2',3'-O-(methoxymethylene)-N-[3-methyl-4-(phosphonooxy)-2-butenyl]-, (E)- (9CI)
(CA INDEX NAME)

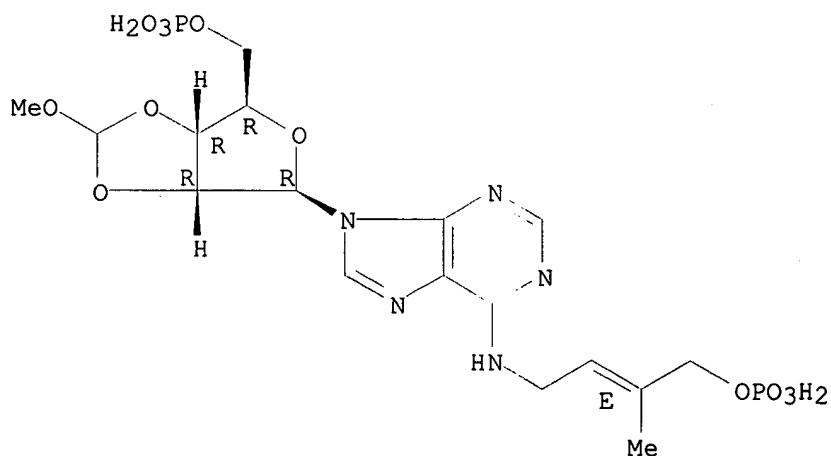
Absolute stereochemistry.
Double bond geometry as shown.



RN 128198-65-2 HCAPLUS

CN 5'-Adenylic acid, 2',3'-O-(methoxymethylene)-N-[3-methyl-4-(phosphonooxy)-2-butenyl]-, (E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



IT 128184-97-4P 128184-98-5P

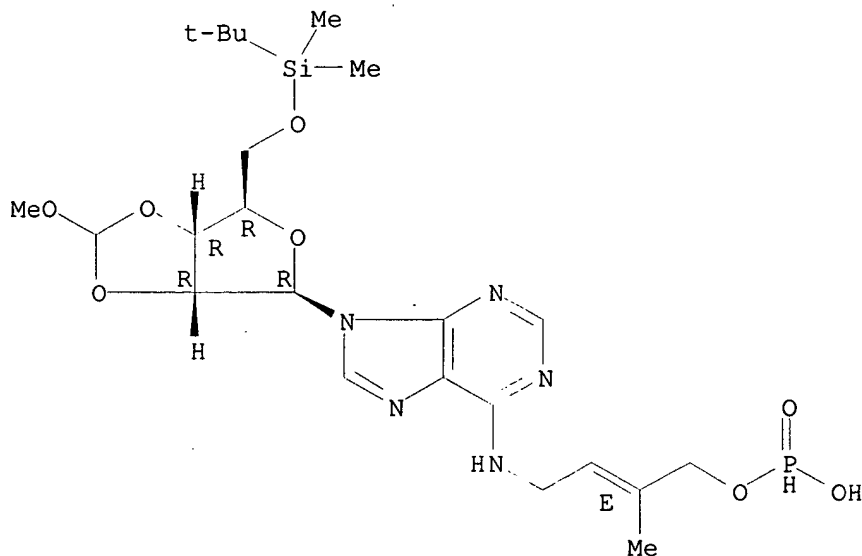
Searched by: Mary Hale 308-4258 CM-1 1E01

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and sequential silylation and oxidn. of, ribosyl zeatin
phosphate from)

RN 128184-97-4 HCAPLUS

CN Adenosine, 5'-O-[(1,1-dimethylethyl)dimethylsilyl]-N-[4-
[(hydroxyphosphinyl)oxy]-3-methyl-2-butenyl]-2',3'-O-(methoxymethylene)-,
(E)- (9CI) (CA INDEX NAME)

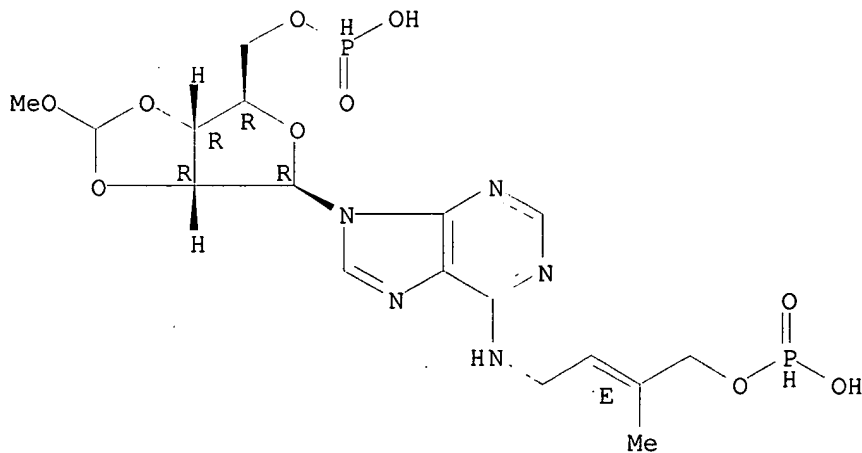
Absolute stereochemistry.
Double bond geometry as shown.



RN 128184-98-5 HCAPLUS

CN Adenosine, N-[4-[(hydroxyphosphinyl)oxy]-3-methyl-2-butenyl]-2',3'-O-
(methoxymethylene)-, 5'-(hydrogen phosphonate), (E)- (9CI) (CA INDEX
NAME)

Absolute stereochemistry.
Double bond geometry as shown.



IT 128059-49-4P 128059-50-7P 128185-00-2P
128185-01-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

Searched by: Mary Hale 308-4258 CM-1 1E01

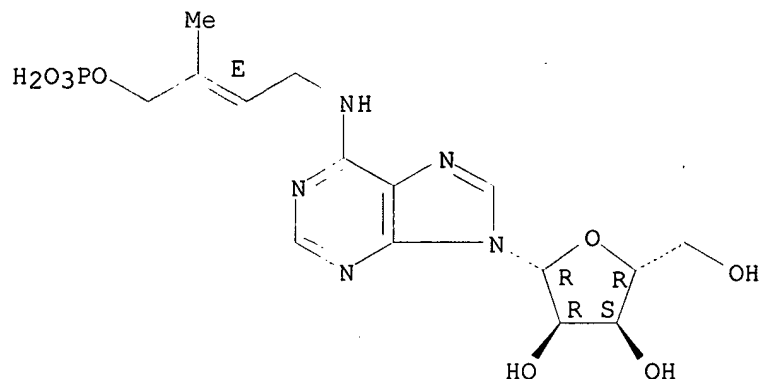
(prepn. of)

RN 128059-49-4 HCAPLUS

CN Adenosine, N-[3-methyl-4-(phosphonoxy)-2-butenyl]-, sodium salt, (E)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



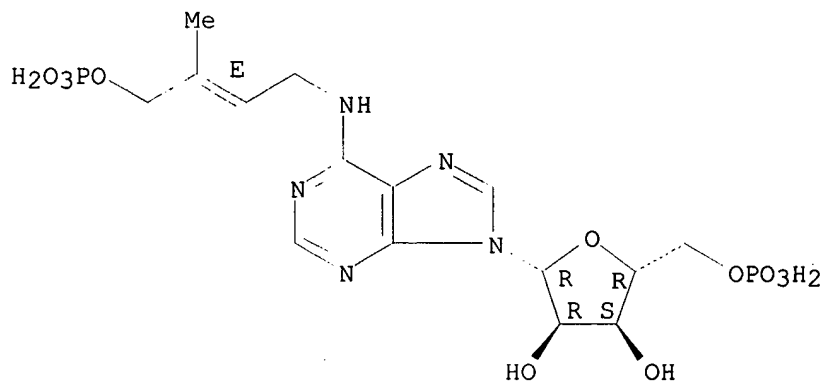
● x Na

RN 128059-50-7 HCAPLUS

CN 5'-Adenylic acid, N-[3-methyl-4-(phosphonoxy)-2-butenyl]-, sodium salt,
(E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



● x Na

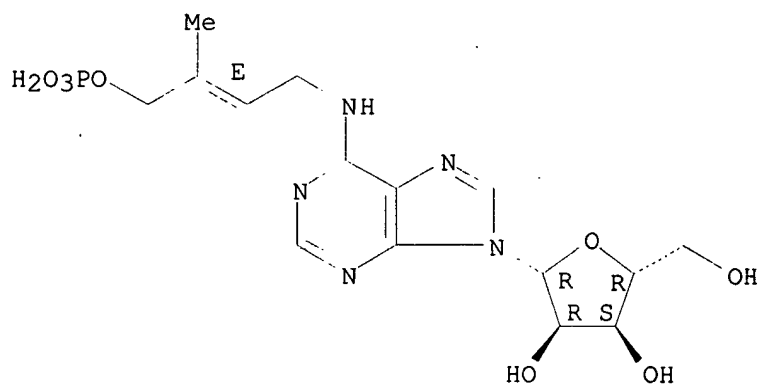
RN 128185-00-2 HCAPLUS

CN Adenosine, N-[3-methyl-4-(phosphonoxy)-2-butenyl]-, (E)- (9CI) (CA INDEX
NAME)

Absolute stereochemistry.

Double bond geometry as shown.

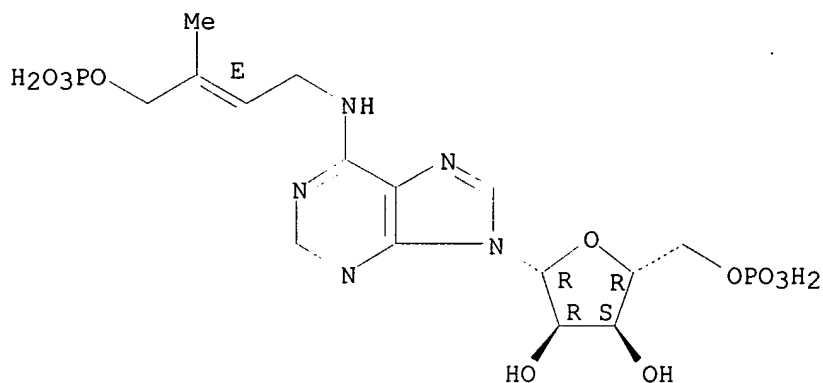
Searched by: Mary Hale 308-4258 CM-1 1E01



RN 128185-01-3 HCAPLUS

CN 5'-Adenylic acid, N-[3-methyl-4-(phosphonooxy)-2-butenyl]-, (E)- (9CI)
(CA INDEX NAME)

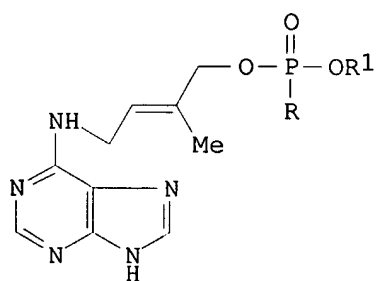
Absolute stereochemistry.
Double bond geometry as shown.



L7 ANSWER 28 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1990:458779 Document No. 113:58779 A convenient new synthesis of the allylic pyrophosphate of trans-zeatin. Shadid, Belal; Van der Plas, Henk C. (Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.). Tetrahedron, 46(3), 895-900 (English) 1990. CODEN: TETRAB. ISSN: 0040-4020. OTHER SOURCES: CASREACT 113:58779.

GI



I

Searched by: Mary Hale 308-4258 CM-1 1E01

AB trans-Zeatin phosphonate I (R = R1 = H) was converted into the phosphoromorpholidate, which on treatment with the Bu3NOP(O)(OH)2 gave the allylic pyrophosphate I [R = OH, R1 = P(O)(OH)2].

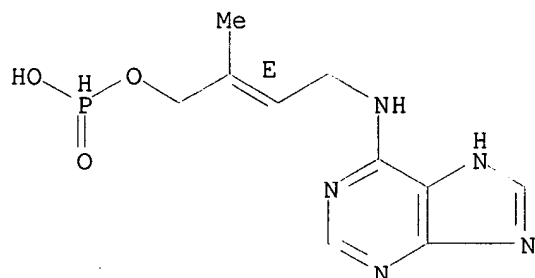
IT 128429-12-9

RL: PROC (Process)
(conversion of, to morpholide)

RN 128429-12-9 HCAPLUS

CN Phosphonic acid, [2-methyl-4-(1H-purin-6-ylamino)-2-butenyl] ester, monosodium salt, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



● Na

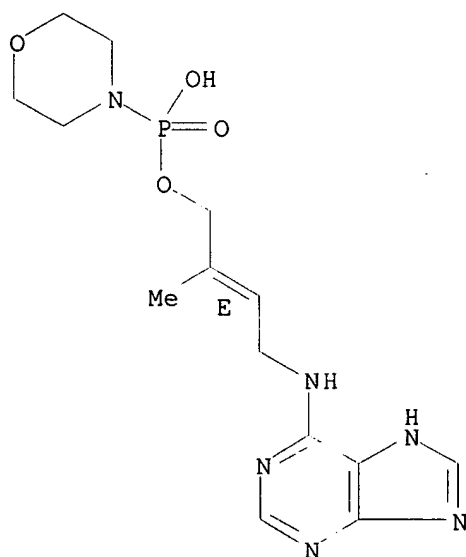
IT 128429-13-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and phosphorylation of)

RN 128429-13-0 HCAPLUS

CN Phosphonic acid, 4-morpholinyl-, mono[2-methyl-4-(1H-purin-6-ylamino)-2-butenyl] ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



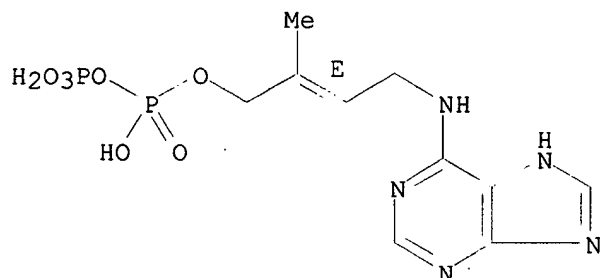
IT 128429-14-1P 128429-15-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

Searched by: Mary Hale 308-4258 CM-1 1E01

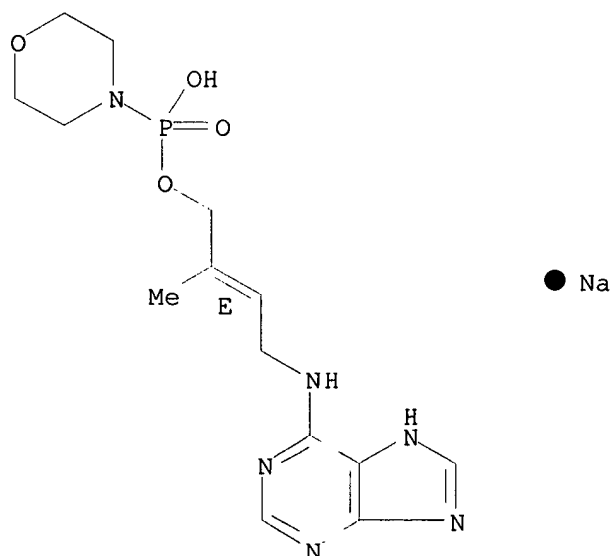
RN 128429-14-1 HCAPLUS
CN Diphosphoric acid, mono[2-methyl-4-(1H-purin-6-ylamino)-2-butenyl] ester,
(E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 128429-15-2 HCAPLUS
CN Phosphonic acid, 4-morpholinyl-, mono[2-methyl-4-(1H-purin-6-ylamino)-2-butenyl] ester, monosodium salt, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L7 ANSWER 29 OF 77 HCAPLUS COPYRIGHT 2002 ACS
1990:420657 Document No. 113:20657 Conditions for the production of agrocin 84 by Agrobacterium radiobacter K84. Formica, Joseph V. (Dep. Microbiol. Immunol., Virginia Commonw. Univ., Richmond, VA, USA). J. Ind. Microbiol., 5(1), 33-44 (English) 1990. CODEN: JIMIE7. ISSN: 0169-4146.
AB A chem. defined medium was developed that supported the growth of A. radiobacter K84 and the prodn. of agrocin 84. Various supplements were investigated for their effect on growth rate and prodn. of agrocin 84 using a well-diffusion assay method. Mannitol was a better substrate for growth of A. radiobacter K84 than the other sugar alcs. and sugars tested. By contrast, D-fructose was the better substrate for the prodn. of agrocin 84. Biotin supplementation stimulated prodn. of agrocin 84 but did not eliminate the diauxic lag seen with the basal medium. The opine octopine inhibited growth of A. radiobacter K84 and prodn. of agrocin 84, as did coenzyme B12. By contrast, the cytokinin isopentenyl adenosine was

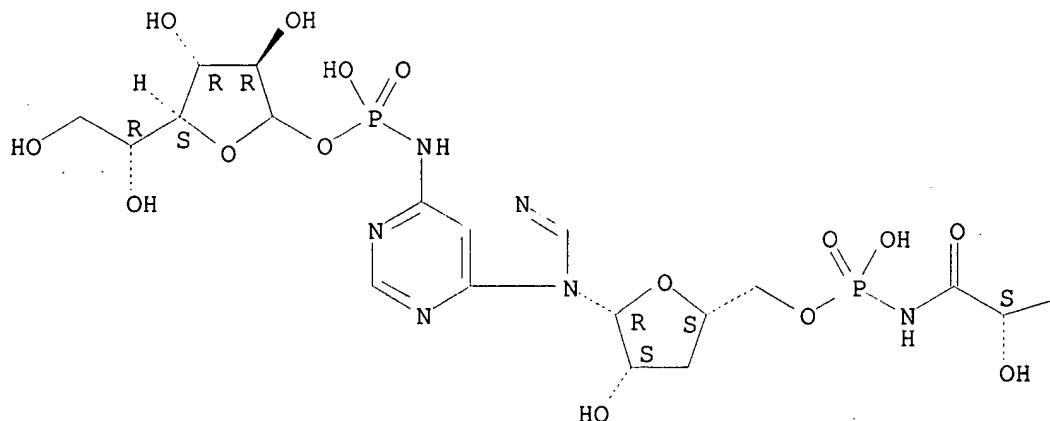
Searched by: Mary Hale 308-4258 CM-1 1E01

IT 59111-78-3, Agrocine 84

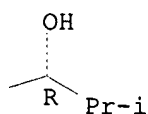
(formation of, by *Agrobacterium radiobacter*)

CN D-Glucufuranose, 1-[hydrogen [9-[3-deoxy-5-O-[[(4,5-dideoxy-4-methyl-D-threo-pentonoyl) amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



1990:52323 Document No. 112:52323 Formation of zeatin allylic phosphate by the microsomal fractions of bulb disks of *Iris .times. hollandica* Tub. and tubers of *Helianthus tuberosus* L. Vonk, C. R.; Davelaar, E.; Ribot, S. A.; Shadid, B.; Van der Plas, H. C. (Cent. Agrobiol. Res., Wageningen, 6700 AA, Neth.). Plant Growth Regul., 8(3), 263-76 (English) 1989. CODEN: PGRED3. ISSN: 0167-6903.

Searched by: Mary Hale 308-4258 CM-1 1E01

partially purified. 5'-AMP was found to be a phosphate group-delivering substrate. Adenosine and adenine inhibited the enzyme reaction. The significance of the results is discussed in relation to cytokinin biosynthesis and the occurrence of bud blast in Iris.

IT 124031-41-0

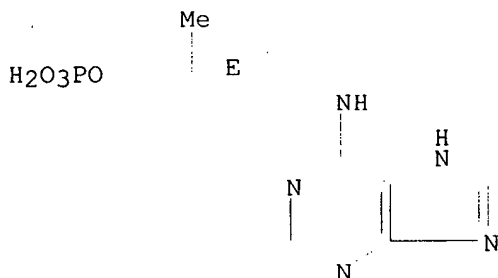
RL: FORM (Formation, nonpreparative)

(formation of, by *Helianthus tuberosus* and iris bulbs, mechanism of)

RN 124031-41-0 HCAPLUS

CN 2-Buten-1-ol, 2-methyl-4-(1H-purin-6-ylamino)-, dihydrogen phosphate (ester), (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L7 ANSWER 31 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1990:17353 Document No. 112:17353 *Agrobacterium* containing transfer-preventing agrocin 84 gene and plasmid therefor in controlling crown gall diseases in plant. Kerr, Allen; Jones, David Allen; Clare, Bruce Garnet; Ryder, Maarten Harm; Farrand, Stephen Kendall (Luminis Pty. Ltd., Australia). Eur. Pat. Appl. EP 313333 A2 19890426, 17 pp. DESIGNATED STATES: R: DE, ES, FR, GB, GR, IT, NL. (English). CODEN: EPXXDW. APPLICATION: EP 1988-309807 19881019. PRIORITY: AU 1987-4977 19871020.

AB Crown gall diseases in plants are controlled by infecting the plant with non-pathogenic *A. radiobacter* contg. a transfer region-deletion plasmid encoding the agrocin 84 gene. Plasmid DAJ102 contg. the agrocin 84 gene without the transfer region was cloned from a BamHI library of pAgK84 and conjugatively transferred into *Agrobacterium* to obtain pAgK1026. The pAgK1026 stably remained in *Agrobacterium* after 10 subcultures; the transfer ability of pAgK1026 was 2-3 order lower than that of transfer region-contg. counterpart, pAgK84. The field trials for inhibition of tumorigenesis and controlling crown gall of almond seedlings induced by *A. tumefaciens* by plasmid pAgK1026, and pAgK 84 were given.

IT 59111-78-3, Agrocin 84

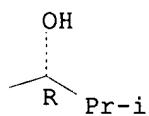
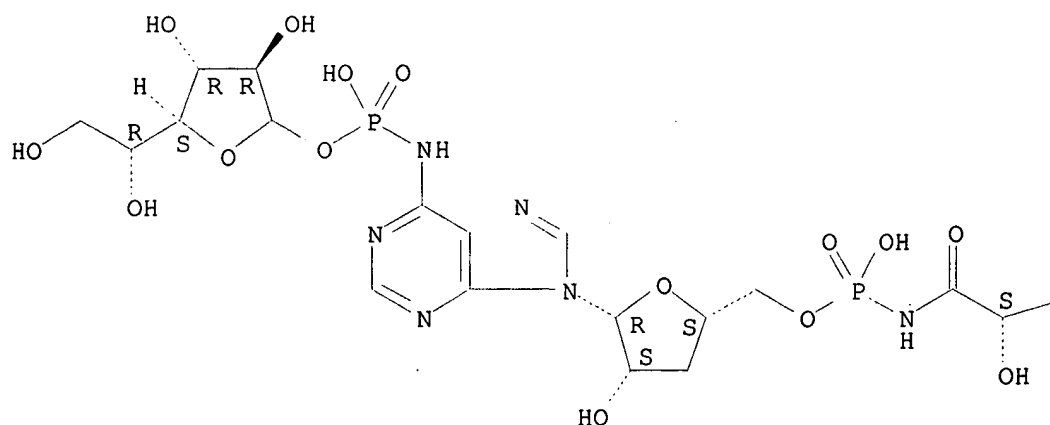
RL: PRP (Properties)

(gene for, cloning and expression in *Agrobacterium radiobacter* of, transfer region-deletion plasmid for)

RN 59111-78-3 HCAPLUS

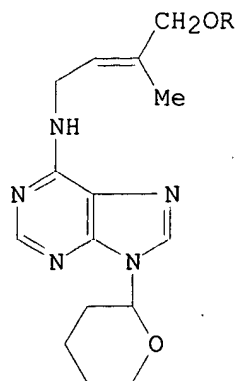
CN D-Glucofuranose, 1-[hydrogen [9-[3-deoxy-5-O-[(4,5-dideoxy-4-methyl-D-threo-pentonoyl)amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 32 OF 77 HCAPLUS COPYRIGHT 2002 ACS
 1990:7250 Document No. 112:7250 The synthesis of allylic phosphate derivatives of trans zeatin. Shadid, Belal; Van der Plas, Henk C.; Vonk, C. R.; Davelaar, E.; Ribot, S. A. (Lab. Org. Chem., Agric. Univ. Wageningen, Wageningen, 6703 HB, Neth.). Tetrahedron, 45(12), 3889-96 (English) 1989. CODEN: TETRAB. ISSN: 0040-4020. OTHER SOURCES: CASREACT 112:7250.

GI



I

AB Phosphitylation of the allylic hydroxy group in 9-tetrahydropyranyl trans-zeatin (I, R = H) with salicyl chlorophosphite gives the allyl phosphonate I [R = P(O)(OH)H], which can be readily converted into I [R = P(S)(OH)2, P(O)(OMe)(OH), P(O)(OH)2]. After cleavage of the tetrahydropyranyl group under mild acidic conditions, allylic phosphate derivs. of trans-zeatin are obtained.

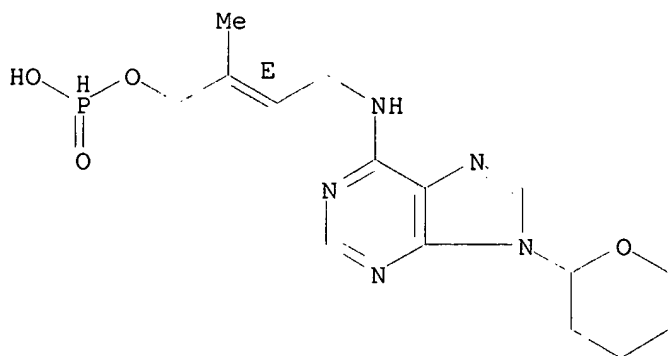
IT 124031-38-5P 124031-40-9P 124031-42-1P
124031-44-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and ether cleavage of)

RN 124031-38-5 HCAPLUS

CN Phosphonic acid, mono[2-methyl-4-[[9-(tetrahydro-2H-pyran-2-yl)-9H-purin-6-yl]amino]-2-butenyl] ester, disodium salt, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

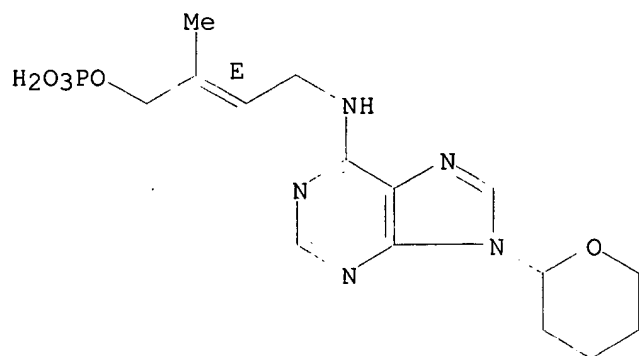


●2 Na

RN 124031-40-9 HCAPLUS

CN 2-Buten-1-ol, 2-methyl-4-[[9-(tetrahydro-2H-pyran-2-yl)-9H-purin-6-yl]amino]-, dihydrogen phosphate (ester), disodium salt, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

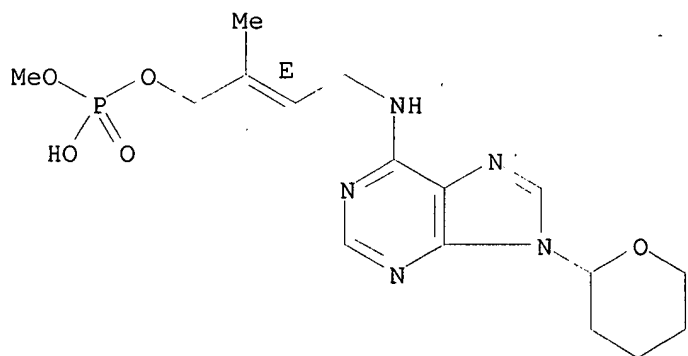


● 2 Na

RN 124031-42-1 HCAPLUS

CN Phosphoric acid, monomethyl mono[2-methyl-4-[[9-(tetrahydro-2H-pyran-2-yl)-9H-purin-6-yl]amino]-2-butenyl] ester, monosodium salt, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

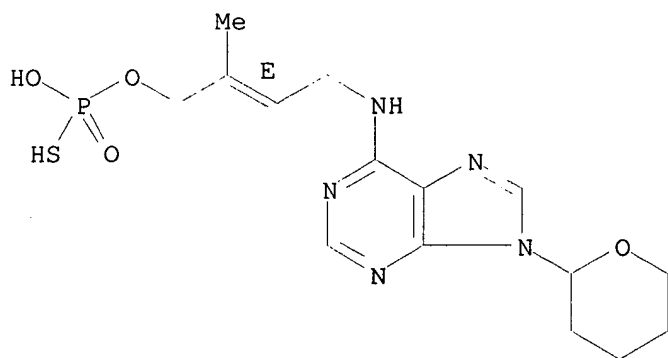


● Na

RN 124031-44-3 HCAPLUS

CN 2-Buten-1-ol, 2-methyl-4-[[9-(tetrahydro-2H-pyran-2-yl)-9H-purin-6-yl]amino]-, dihydrogen phosphorothioate (ester), disodium salt, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



● 2 Na

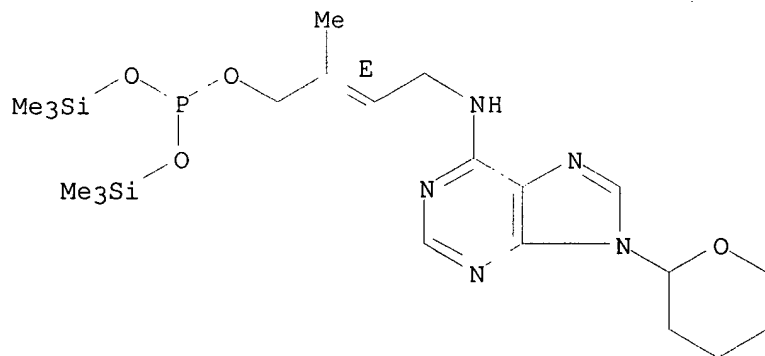
IT 124031-39-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, with dipyridyl disulfide)

RN 124031-39-6 HCAPLUS

CN Phosphorous acid, 2-methyl-4-[[9-(tetrahydro-2H-pyran-2-yl)-9H-purin-6-yl]amino]-2-butenyl bis(trimethylsilyl) ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



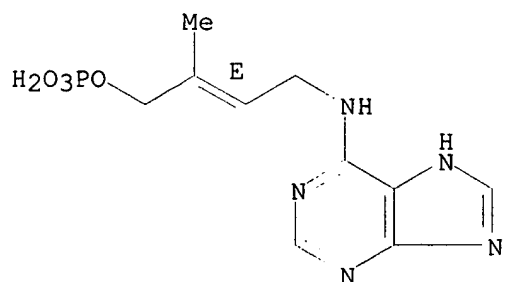
IT 124031-41-0P 124031-43-2P 124031-45-4P
124061-45-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 124031-41-0 HCAPLUS

CN 2-Buten-1-ol, 2-methyl-4-(1H-purin-6-ylamino)-, dihydrogen phosphate
(ester), (2E)- (9CI) (CA INDEX NAME)

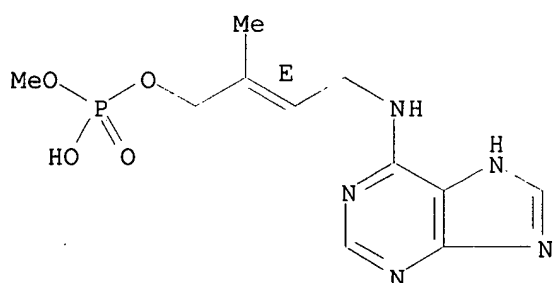
Double bond geometry as shown.



RN 124031-43-2 HCAPLUS

CN Phosphoric acid, monomethyl mono[2-methyl-4-(1H-purin-6-ylamino)-2-butenyl] ester, (E)- (9CI) (CA INDEX NAME)

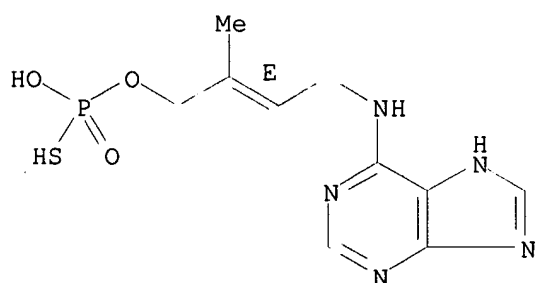
Double bond geometry as shown.



RN 124031-45-4 HCAPLUS

CN 2-Buten-1-ol, 2-methyl-4-(1H-purin-6-ylamino)-, dihydrogen phosphorothioate (ester), (E)- (9CI) (CA INDEX NAME)

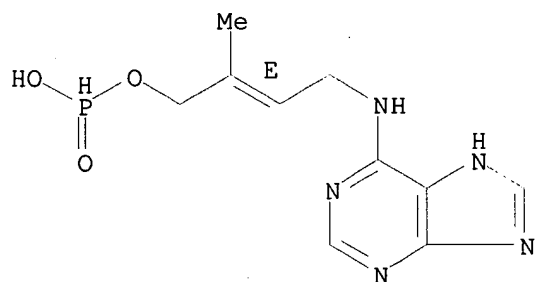
Double bond geometry as shown.



RN 124061-45-6 HCAPLUS

CN Phosphonic acid, mono[2-methyl-4-(1H-purin-6-ylamino)-2-butenyl] ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L7 ANSWER 33 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1989:626076 Document No. 111:226076 Negative effects of agrocin 84-encoding Agrobacterium plasmids on symbiotic properties of Rhizobium meliloti. Law, Ian J.; Strijdom, Barend W. (Plant Prot. Res. Inst., Pretoria, 0001, S. Afr.). Arch. Microbiol., 152(5), 463-7 (English) 1989. CODEN: AMICCW. ISSN: 0302-8933.

AB Two plasmids, pAgK84::Tn5-Mob from Agrobacterium radiobacter carrying genes for the prodn. of agrocin 84, and RP4-4 from Escherichia coli, were inserted either sep. or together into a strain of Rhizobium meliloti. Each of these plasmid-contg. R. meliloti transconjugants was less effective than the wild type strain in their ability to fix nitrogen in Medicago tornata. The pAgK84::Tn5-Mob-contg. transconjugant was significantly less effective than that contg. RP4-4. The transconjugant strains were inferior to the wild type strain in their ability to nodulate seedlings and to compete for nodulation.

IT 59111-78-3, Agrocin 84

RL: PRP (Properties)

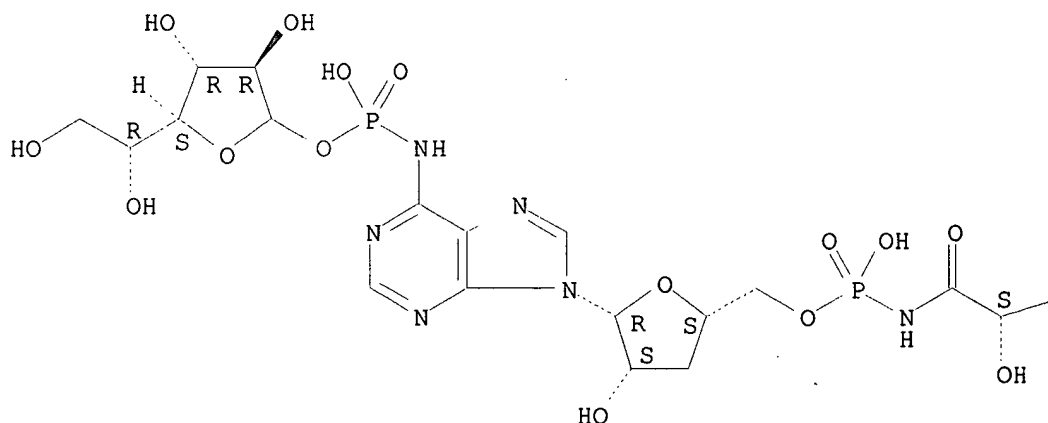
(plasmid of Agrobacterium radiobacter encoding, neg. effect of, on symbiotic properties of Rhizobium meliloti)

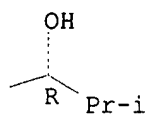
RN 59111-78-3 HCAPLUS

CN D-Glucufuranose, 1-[hydrogen [9-[3-deoxy-5-O-[[[4,5-dideoxy-4-methyl-D-threo-pentonoyl)amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

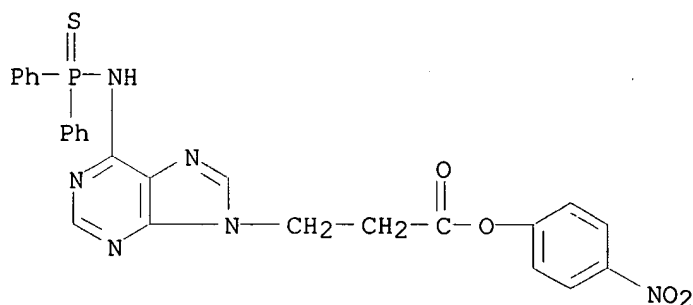
Absolute stereochemistry.

PAGE 1-A





- L7 ANSWER 34 OF 77 HCAPLUS COPYRIGHT 2002 ACS
 1989:595537 Document No. 111:195537 Functional monomers and polymers. CLIV. Application of nucleic acid base containing polymers to high-performance liquid chromatography. Nagae, Suguru; Suda, Yasuo; Inaki, Yoshiaki; Takemoto, Kiichi (Fac. Eng., Osaka Univ., Suita, 565, Japan). J. Polym. Sci., Part A: Polym. Chem., 27(8), 2593-609 (English) 1989. CODEN: JPACEC. ISSN: 0887-624X.
- AB Poly(L-lysine) derivs. contg. pendant nucleic acid bases, such as thymine or adenine, were bonded successfully to 3-aminopropylsilanized silica and silica gel. These resins were useful as the column of HPLC for the selective sepn. of oligoethylenimine derivs. having pendant thymine or adenine bases.
- IT **123549-43-9DP**, reaction products with brominated poly(carbobenzyloxylysine)
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
- RN 123549-43-9 HCAPLUS
- CN 9H-Purine-9-propanoic acid, 6-[(diphenylphosphinothioyl)amino]-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)



- L7 ANSWER 35 OF 77 HCAPLUS COPYRIGHT 2002 ACS
 1989:149747 Document No. 110:149747 Evidence of biological control of Agrobacterium tumefaciens strains sensitive and resistant to agrocin 84 by different Agrobacterium radiobacter strains on stone fruit trees. Lopez, Maria M.; Gorris, Maria Teresa; Salcedo, Carmina I.; Montojo, Ana M.; Miro, Marcela (Inst. Valenciano Invest. Agrar., Valencia, Spain). Appl. Environ. Microbiol., 55(3), 741-6 (English) 1989. CODEN: AEMIDF. ISSN: 0099-2240.
- AB The effectiveness of A. radiobacter K84, 0341, and K84 non-agrocin-producing mutant (K84 Agr-) in biol. control of crown gall on

rootstocks of stone fruit trees was detd. in three expts. In expt. 1, K84 and 0341 controlled crown gall on plum plants in soil inoculated with two strains of *A. tumefaciens* resistant to agrocin 84. In expt. 2, K84 controlled crown gall on peach plants in soils inoculated with strains of *A. tumefaciens* sensitive or resistant to agrocin 84 or with a mixt. of both. However, the effectiveness of K84 was higher against the sensitive strain than against the resistant strain. There was a residual effect of K84 from one year to another in soil inoculated with the sensitive strains. In expt. 3, K84 and K84 Agr- controlled crown gall on plum and peach plants in soils inoculated with strains of *A. tumefaciens* sensitive or resistant to agrocin 84. The control afforded by K84 was higher than that provided by K84 Agr- against the sensitive strain but was similar against the resistant strain.

IT 59111-78-3, Agrocin 84

RL: BIOL (Biological study)

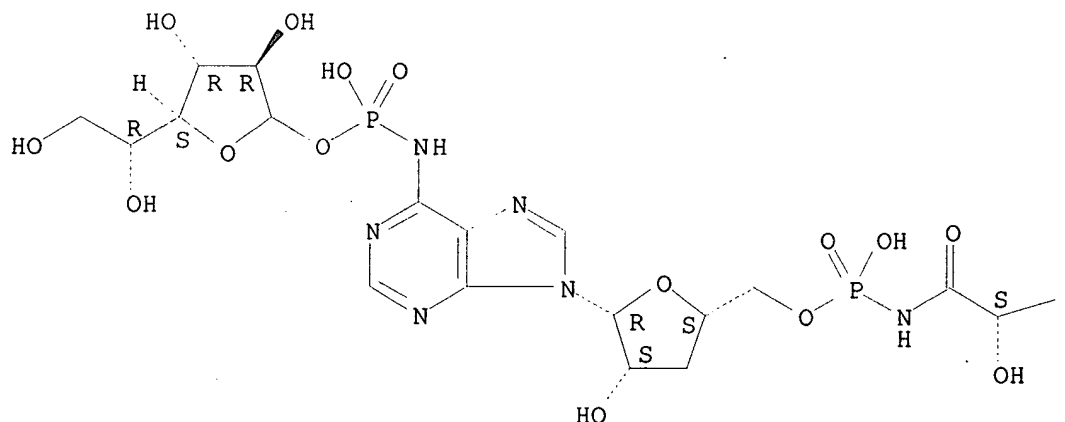
(*Agrobacterium tumefaciens* resistance to, crown gall of plum and peach control by *A. radiobacter* in relation to)

RN 59111-78-3 HCAPLUS

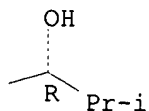
CN D-Glucofuranose, 1-[hydrogen [9-[3-deoxy-5-O-[[[4,5-dideoxy-4-methyl-D-threo-pentonoyl]amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



L7 ANSWER 36 OF 77 HCAPLUS COPYRIGHT 2002 ACS

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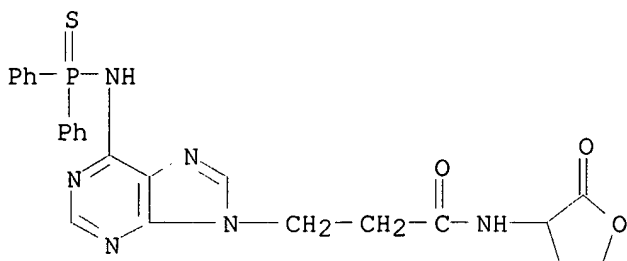
1989:95944 Document No. 110:95944 Functional monomers and polymers. CLXXII. Synthesis and interaction studies on water-soluble nucleic acid analogs: poly(ethylenimine) derivatives containing thymine and adenine. Wada, Takehiko; Inaki, Yoshiaki; Takemoto, Kiichi (Fac. Eng., Osaka Univ., Suita, 565, Japan). Polym. J. (Tokyo), 20(11), 1059-68 (English) 1988. CODEN: POLJB8. ISSN: 0032-3896.

AB Water-sol. nucleic acid analogs were prepd. by grafting adenine and thymine derivs. with homoserine onto polyethylenimine. The analogs formed complementary polymer complexes with each other and with polynucleotides. The interactions were studied between these polymers, and with polyuridylic acid and polyadenylic acid in water.

IT **119225-18-2DP**, reaction products with polyethylenimine
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and interaction of)

RN 119225-18-2 HCAPLUS

CN 9H-Purine-9-propanamide, 6-[(diphenylphosphinothioyl)amino]-N-(tetrahydro-2-oxo-3-furanyl)- (9CI) (CA INDEX NAME)

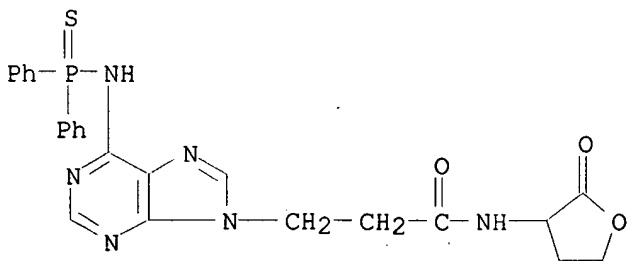


IT **119225-18-2P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, with polyethylenimine)

RN 119225-18-2 HCAPLUS

CN 9H-Purine-9-propanamide, 6-[(diphenylphosphinothioyl)amino]-N-(tetrahydro-2-oxo-3-furanyl)- (9CI) (CA INDEX NAME)

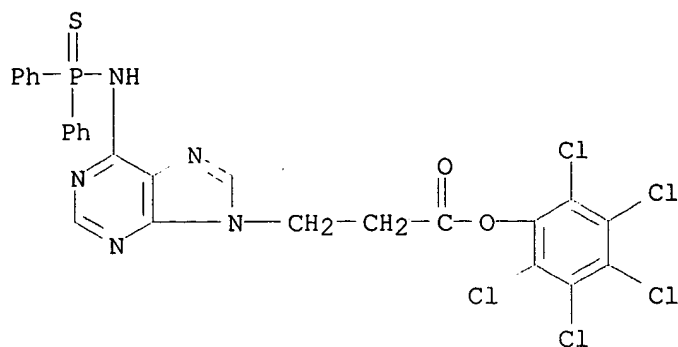


IT **119225-19-3**

RL: RCT (Reactant)
(reaction of, with aminobutyrolactone hydrobromide)

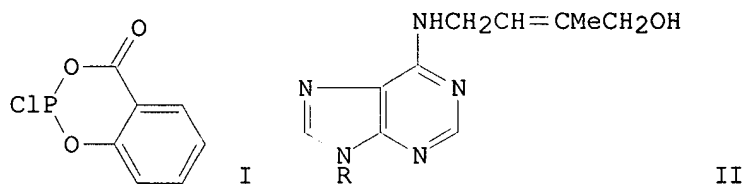
RN 119225-19-3 HCAPLUS

CN 9H-Purine-9-propanoic acid, 6-[(diphenylphosphinothioyl)amino]-, pentachlorophenyl ester (9CI) (CA INDEX NAME)



L7 ANSWER 37 OF 77 HCAPLUS COPYRIGHT 2002 ACS
 1988:493147 Document No. 109:93147 Phosphorylation of allylic hydroxy groups
 via phosphite intermediates. Shadid, B. R.; Van der Plas, H. C.; De
 Vroom, E.; Van der Marel, G. A.; Van Boom, J. H. (Org. Chem. Lab., Agric.
 Univ., Wageningen, 6703 BC, Neth.). Recl. Trav. Chim. Pays-Bas, 106(9),
 509-11 (English) 1987. CODEN: RTCPA3. ISSN: 0165-0513. OTHER SOURCES:
 CASREACT 109:93147.

GI



AB Reaction of an allylic hydroxy group in $RCH_2CH:CHMeCH_2OH$ (R = phthalimide)
 with salicylchlorophosphite I gives an allyl 1-H-phosphonate monoester,
 which can be readily hydrolyzed, silylated, and then oxidized to the
 corresponding phosphate monoester $RCH_2CH:CHMeCH_2OP(O)(OH)_2$. Application of
 this phosphite tri-ester approach was further demonstrated in the prepn.
 of 1-H-phosphonate and phosphate monoesters of N-protected trans-zeatin II
 (R = tetrahydropyranyl).

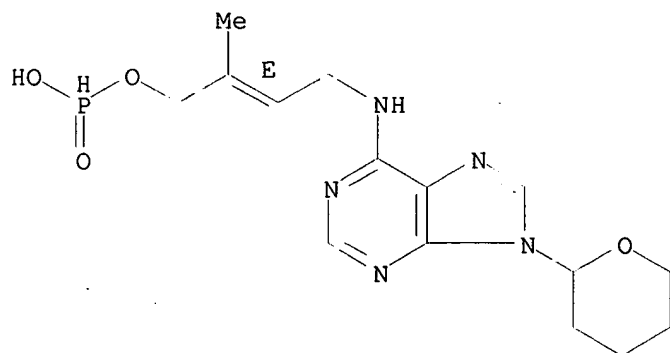
IT 115845-92-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and silylation-oxidn. of, phosphate monoester from)

RN 115845-92-6 HCAPLUS

CN Phosphonic acid, mono[2-methyl-4-[[9-(tetrahydro-2H-pyran-2-yl)-9H-purin-6-yl]amino]-2-butenyl] ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



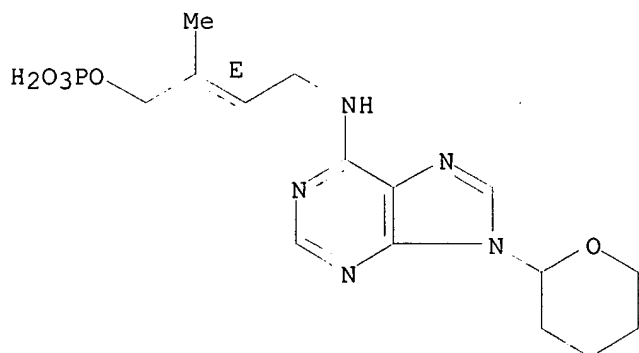
IT 115845-93-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 115845-93-7 HCAPLUS

CN 2-Buten-1-ol, 2-methyl-4-[[9-(tetrahydro-2H-pyran-2-yl)-9H-purin-6-yl]amino]-, dihydrogen phosphate (ester), (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L7 ANSWER 38 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1988:449246 Document No. 109:49246 Construction of a Tra- deletion mutant of pAgK84 to safeguard the biological control of crown gall. Jones, David A.; Ryder, Maarten H.; Clare, Bruce G.; Farrand, Stephen K.; Kerr, Allen (Waite Agric. Res. Inst., Univ. Adelaide, Glen Osmond, 5064, Australia). MGG, Mol. Gen. Genet., 212(2), 207-14 (English) 1988. CODEN: MGGEAE. ISSN: 0026-8925.

AB Agrobacterium radiobacter Strain K84 is used com. for the biol. control of crown gall. It contains the conjugative plasmid pAgK84, which encodes the synthesis of agrocin 84, an antibiotic that inhibits many pathogenic agrobacteria. A breakdown of control is threatened by the transfer of pAgK84 to pathogens, which then become resistant to agrocin 84. A mutant of pAgK84 with a 5.9-kb deletion overlapping the transfer (Tra) region was constructed using recombinant DNA techniques. The BamHI fragment B1 which covers most of the Tra region was cloned in pBR325 and its internal EcoRI fragments D1 and H, which overlap the Tra region, were removed, leaving 3.7 and 0.5 kb of pAgK84 on either side of the deletion. The latter was increased to 3.3 kb by adding EcoRI fragment D2 from a BamHI fragment C clone. The modified pBR325 clone was mobilized into Agrobacterium strain NT1 harboring pAgK84 with a Tn5 insertion just outside the Tra region but covered by the deletion. A Tra+ cointegrate was formed between the

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Tn5-insertion deriv. and the pBR325-based deletion construct by homologous recombination. The cointegrate was transferred by conjugation to a deriv. of strain K84 lacking pAgK84, in which a second recombination event generated a stable deletion-mutant by deletion-marker exchange. The resultant new strain of *A. radiobacter*, designated K1026, shows normal agrocin 84 prodn. Mating expts. show that the mutant plasmid, designated pAgK1026, is incapable of conjugal transfer at a detectable frequency.

IT 59111-78-3, Agrocin 84

RL: FORM (Formation, nonpreparative)

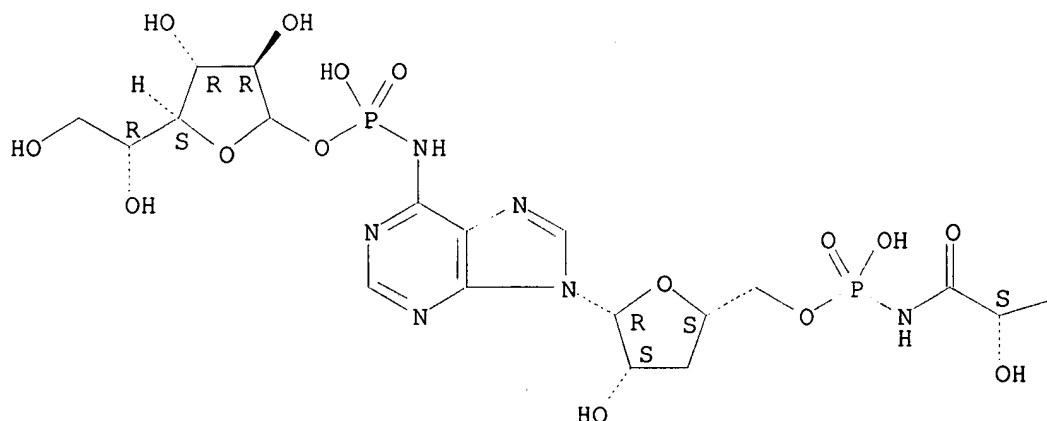
(formation of, by *Agrobacterium radiobacter*, mutation in plasmid pAgK84 in relation to)

RN 59111-78-3 HCAPLUS

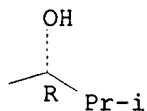
CN D-Glucofuranose, 1-[hydrogen [9-[3-deoxy-5-O-[[[4,5-dideoxy-4-methyl-D-threo-pentonoyl)amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



L7 ANSWER 39 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1988:199064 Document No. 108:199064 Characterization and mapping of the agrocinopine-agrocin 84 locus on the nopaline Ti plasmid pTiC58. Hayman, G. Thomas; Farrand, Stephen K. (Med. Cent., Loyola Univ., Maywood, IL, 60153, USA). *J. Bacteriol.*, 170(4), 1759-67 (English) 1988. CODEN: JOBAAY. ISSN: 0021-9193.

AB Overlapping segments of pTiC58 inserted into cosmid vectors were used to

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characterize the agrocinopine-agrocin 84 locus from the nopaline-agrocinopine A and B *Agrobacterium tumefaciens* strain C58. All of the clones conferring agrocin 84 sensitivity on agrobacteria also conferred uptake of agrocin 84 and agrocinopines A and B. Transposon Tn3-HoHol insertion mutations of one such clone were generated that simultaneously abolished agrocin 84 sensitivity and transport of agrocinopines A and B and agrocin 84. Such insertions were found to cluster within a 4.4-kilbase region. Anal. of .beta.-galactosidase activity in these insertion mutants suggested a single transcriptional unit regulated at the transcriptional level by agrocinopines A and B. The smallest DNA fragment subcloned from the region to confer all 3 activities was 8.5 kilobases long. This subclone was still properly regulated, indicating that the regulatory gene is closely linked to the locus. The data are consistent with a single operon encoding catabolism of agrocinopines A and B and conferring sensitivity to agrocin 84. Based on these results, the locus name acc, for agrocinopine catabolism, was suggested.

IT 59111-78-3, Agrocin 84

RL: PRP (Properties)

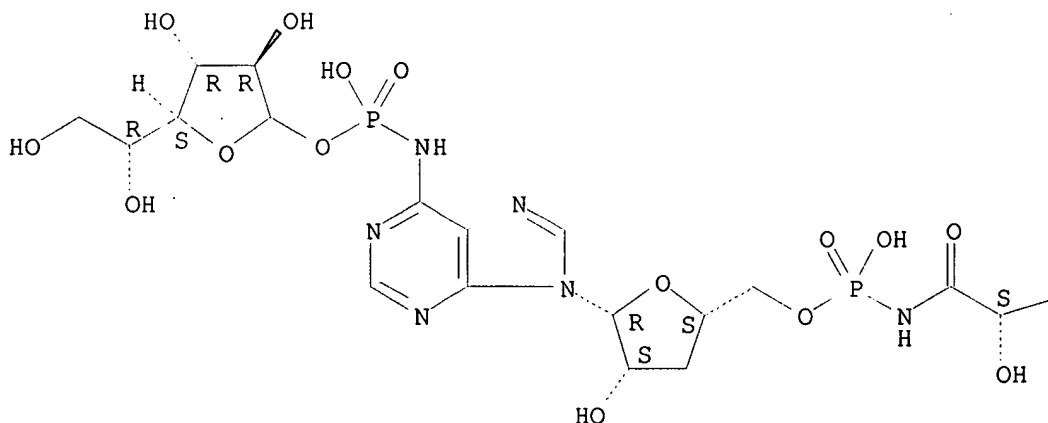
(gene for, of plasma pTiC58, characterization and mapping of)

RN 59111-78-3 HCAPLUS

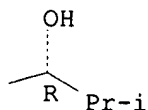
CN D-Glucofuranose, 1-[hydrogen [9-[3-deoxy-5-O-[[(4,5-dideoxy-4-methyl-D-threo-pentonoyl)amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



L7 ANSWER 40 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1988:150897 Document No. 108:150897 Characteristics of ion evaporation ionization in thermospray high performance liquid chromatography/mass spectrometry. Voyksner, Robert D. (Research Triangle Inst., Research Triangle Park, NC, 27709, USA). Org. Mass Spectrom., 22(8), 513-18 (English) 1987. CODEN: ORMSBG. ISSN: 0030-493X.

AB Thermospray ion evapn./mass spectrometry in the absence of buffer or auxiliary ionization techniques can prove useful in detecting org. compds. The ion evapn. process appears to be dependent on the type and relative amt. of ionic species in soln. The best sensitivity was obtained at low pH for fully protonated species. The $[M + H]^+$ and $[M + Na]^+$ ion intensities varied directly with soln. acid and salt concn., resp. This dependence enabled the calcn. of $pK'a$ values from thermospray data. Alkali metal adduct ions were favored at a pH where the analyte was ionized in soln. The adduct ions were formed with most alkali metals and the intensity increased with the stability of the ionic complex ($Li > Na > K > Rb > Cs$). The kinetics for the metal adduct ion were different from the $[M + H]^+$ ion formation. Possibly the formation of the $[M + H]^+$ ions occurred by gas-phase reaction based on proton affinities while the metal adducts were derived from desolvated ionic complexes. Ion evapn. spectra without ammonium acetate resembled the type of spectra acquired from desorption ionization techniques (fast atom bombardment). It appears that ion evapn. without buffer is dependent on soln. chem. The addn. of ammonium acetate reduced soln. phase dependence, so the spectra were not changed by the pH.

IT 113729-33-2

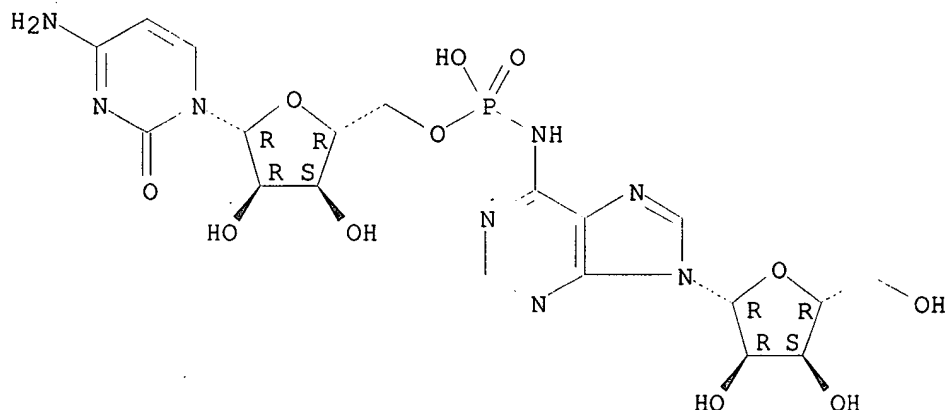
RL: PRP (Properties)

(ion evapn. spectra of, analyzed by thermospray HPLC/MS)

RN 113729-33-2 HCAPLUS

CN Adenosine, N-5'-cytidyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 41 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1988:17885 Document No. 108:17885 Peroxisomal .beta.-oxidation of long-chain fatty acids possessing different extents of unsaturation. Hovik, Rolf; Osmundsen, Harald (Dent. Sch., Univ. Oslo, Oslo, 0316, Norway). Biochem. J., 247(3), 531-5 (English) 1987. CODEN: BIJOAK. ISSN: 0306-3275.

AB Rates of peroxisomal .beta.-oxidn. were measured as fatty acyl-CoA-dependent NAD redn. in solubilized peroxisomal fractions isolated from livers of rats treated with clofibrate. Medium- to long-chain satd. fatty acyl-CoA esters as well as long-chain polyunsatd. fatty acyl-CoA

Searched by: Mary Hale 308-4258 CM-1 1E01

IT 111846-63-0P

RN 111846-63-0 HCAPLUS

CN	Coenzyme A, S-11-docosenoate (9CI)	(CA INDEX NAME)
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NC1=NC=NC2=C1N=CN2[C@@H]3O[C@H](COP(=O)(O)OP(=O)(O)OCC(C)(C)C(O)C(=O)NCC)[C@H](O)[C@@H](O)[C@H]3O
$$-\text{CH}_2-\overset{\overset{\text{O}}{\parallel}}{\text{C}}-\text{NH}-\text{CH}_2-\text{CH}_2-\text{S}-\overset{\overset{\text{O}}{\parallel}}{\text{C}}-(\text{CH}_2)_9-\text{CH}=\text{CH}-(\text{CH}_2)_9-\text{Me}$$

1987:569607 Document No. 107:169607 Genetics and molecular biology of
agrocin production and sensitivity in *Agrobacterium*. Farrand, S. K.;
Ryder, M. H.; Hayman, G. T.; O'Morchoe, S. B.; Shim, J. S.; Kerr, Allen
(Dep. Microbiol., Stritch Sch. Med., Maywood, IL, 60153, USA). Plant
Pathog. Bact., Proc. Int. Conf., 6th, Meeting Date 1985, 42-55.
Editor(s): Civerolo, E. L. Nijhoff: Dordrecht, Neth. (English) 1987.
CODEN: 55ZVAG.

Searched by: Mary Hale 308-4258 CM-1 1E01

Cosmid clones of this Ti plasmid were isolated which confer agrocin 84 sensitivity on a Ti plasmidless *A. tumefaciens* strain. Strains harboring such cosmid clones are capable of transporting agrocinopine A. Anal. of cosmid overlaps and also of transposon insertions confines the agrocin sensitivity locus to a 6-kb region of the Ti plasmid.

IT 59111-78-3, Agrocin 84

RL: PRP (Properties)

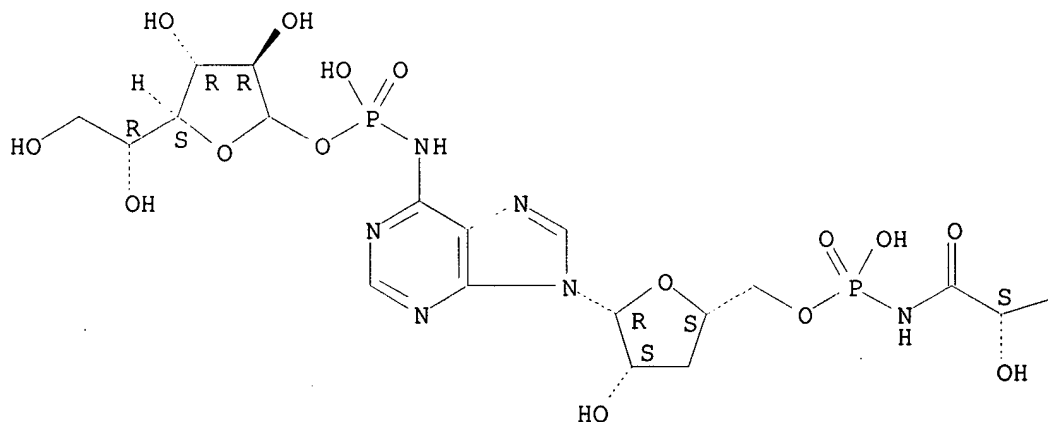
(formation of and sensitivity to, in *Agrobacterium radiobacter*, genetics and mol. biol. of)

RN 59111-78-3 HCAPLUS

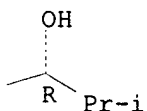
CN D-Glucofuranose, 1-[hydrogen [9-[3-deoxy-5-O-[[[(4,5-dideoxy-4-methyl-D-threo-pentonoyl)amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



L7 ANSWER 43 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1987:548229 Document No. 107:148229 Genetic analysis of agrocin 84 production and immunity in *Agrobacterium* spp. Ryder, Maarten H.; Slota, John E.; Scarim, Anna; Farrand, Stephen K. (Stritch Sch. Med., Loyola Univ. Chicago, Maywood, IL, 60153, USA). *J. Bacteriol.*, 169(9), 4184-9 (English) 1987. CODEN: JOBAAY. ISSN: 0021-9193.

AB Mutations affecting agrocin prodn. on the 48-kilobase (kb) plasmid, pAgK84, can be complemented in trans with cloned portions of the plasmid. Five complementation groups ranging in min. size from 1.2 to 5.6 kb were

Searched by: Mary Hale 308-4258 CM-1 1E01

identified within a 15-kb segment. Plasmid pAgK84-encoded immunity to agrocin 84 was located to 2 sep. regions of the plasmid. Either region alone was sufficient to protect sensitive strains, and both loci mapped to the agrocin 84 biosynthesis region. One region is located within complementation group I, whereas the other forms a part of complementation group IV. Prodn. of agrocin 84 was unaffected by nopaline, agrocinopine A, acetosyringone, or low or high levels of ferric iron. Agrocin 84 prodn. was greatly suppressed when the strain also contained a Ti plasmid nutritionally or mutationally derepressed for agrocinopine A catabolism. RNA dot-blot anal. indicated that decreased agrocin 84 prodn. by such strains was not due to transcriptional repression of agrocin 84 biosynthetic loci. In strains also harboring pAtK84b, the opine catabolic plasmid of *A. radiobacter* K84, induction of the agrocinopine A catabolic locus of this plasmid had no such effect on agrocin 84 prodn.

IT 59111-78-3, Agrocin 84

RL: PRP (Properties)

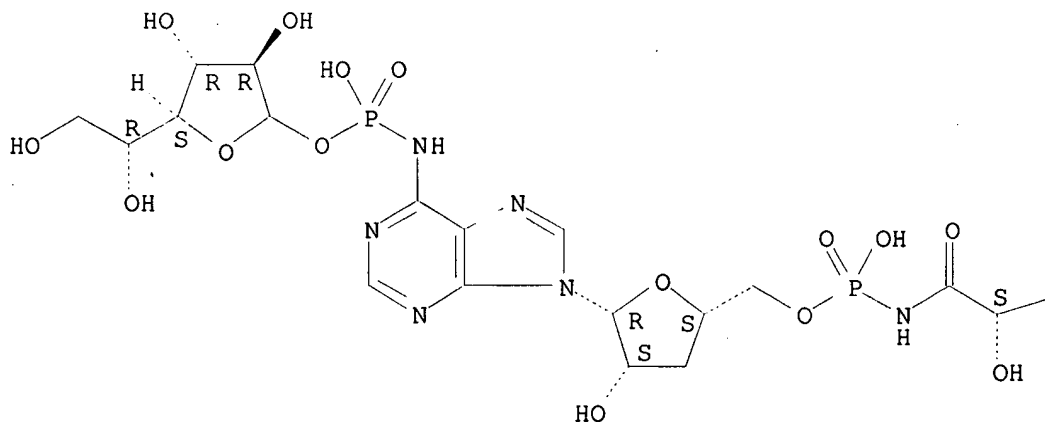
(formation of and immunity to, in *Agrobacterium*, genetic anal. of)

RN 59111-78-3 HCAPLUS

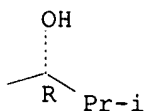
CN D-Glucofuranose, 1-[hydrogen [9-[3-deoxy-5-O-[[[4,5-dideoxy-4-methyl-D-threo-pentonoyl]amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



1987:455639 Document No. 107:55639 Sensitivity of different *Agrobacterium* strains to agrocin 84. Ondrej, M.; Vlasak, J. (Inst. Exp. Bot., Czech. Acad. Sci., Ceske Budejovice, 370 05, Czech.). *Folia Microbiol.* (Prague), 32(3), 239-43, 1 plate (English) 1987. CODEN: FOMIAZ. ISSN: 0015-5632.

AB Sensitivity of 14 *A. tumefaciens* and *A. rhizogenes* strains to agrocin 84 was followed. A new agrocin 84 sensitivity of mannopine strains of *A. rhizogenes* 8196 and TR101 was described. Agropine strains of *A. rhizogenes* and *A. tumefaciens* were also sensitive to agrocin 84. Agrocin 84 sensitivity of succinamopine and mannopine strains of *A. tumefaciens* was also confirmed.

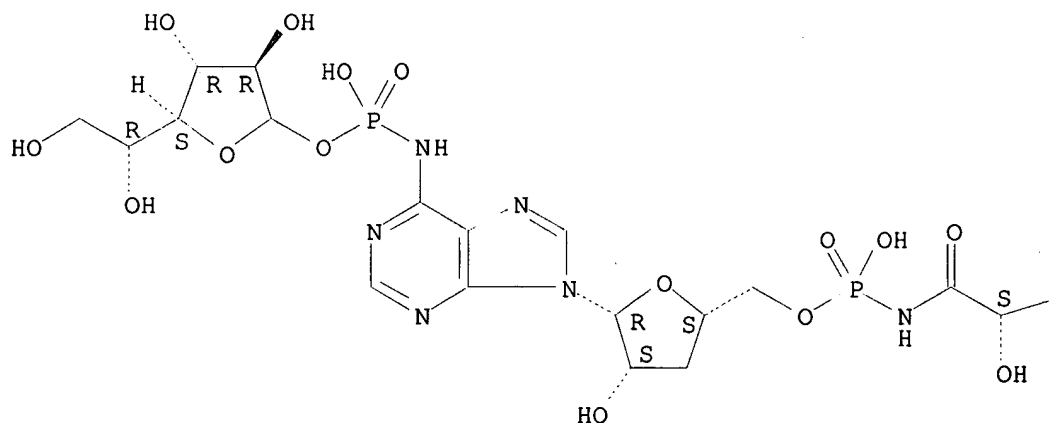
IT 59111-78-3, Agrocin 84
 RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)
 (Agrobacterium sensitivity to)

RN 59111-78-3 HCAPLUS

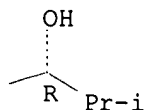
CN D-Glucofuranose, 1-[hydrogen [9-[3-deoxy-5-O-[[[(4,5-dideoxy-4-methyl-D-threo-pentonoyl)amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



L7 ANSWER 45 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1987:132408 Document No. 106:132408 Tn5 insertions in the agrocin 84 plasmid: the conjugal nature of pAgK84 and the locations of determinants for transfer and agrocin 84 production. Shim, Jae Sup (Coll. Agric.,

Searched by: Mary Hale 308-4258 CM-1 1E01

Chungbuk Univ., S. Korea). Misaengmul kwa Sanop, 12(2), 2-13 (Korean) 1986. CODEN: MKSAEQ.

AB A review with 43 refs.

IT 59111-78-3

RL: BIOL (Biological study)

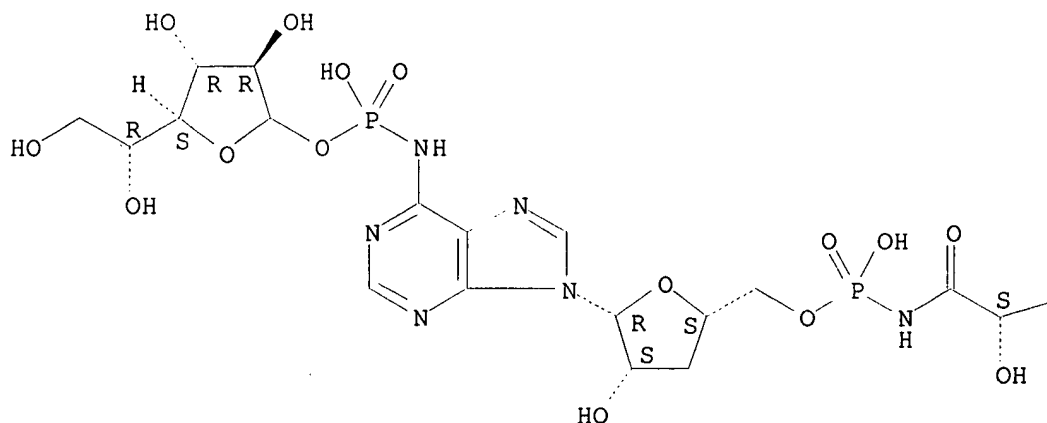
(plasmid-mediated formation of, by *Agrobacterium tumefaciens*,
transposon insertion in relation to)

RN 59111-78-3 HCAPLUS

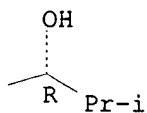
CN D-Glucofuranose, 1-[hydrogen [9-[3-deoxy-5-O-[[(4,5-dideoxy-4-methyl-D-threo-pentonoyl)amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



L7 ANSWER 46 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1987:44705 Document No. 106:44705 A spontaneous insertion in the agrocin sensitivity region of the Ti-plasmid of *Agrobacterium tumefaciens* C58. Cooksey, Donald A. (Dep. Plant Pathol., Univ. California, Riverside, CA, 92521, USA). Plasmid, 16(3), 222-4 (English) 1986. CODEN: PLSDMX. ISSN: 0147-619X.

AB A spontaneous agrocin-resistant mutant of *A. tumefaciens* strain C58 had an insertion of 1.2 kb in the agrocin sensitivity region of pTiC58. The insertion was cloned from the Ti plasmid, and a subclone contg. only DNA internal to the insertion was used to probe the Ti plasmid and chromosomal DNA of the wild-type strain C58. The probe showed homol. to chromosomal

Searched by: Mary Hale 308-4258 CM-1 1E01

sequences but showed no homol. to wild-type pTiC58. Homol. was also detected with chromosomal sequences of *A. tumefaciens* strains B6, K24, and T37. These results suggest that an indigenous insertion sequence of 1.2 kb transposed from the chromosome to the agrocin sensitivity region of the Ti plasmid in this spontaneous mutant of C58.

IT 59111-78-3

RL: PRP (Properties)

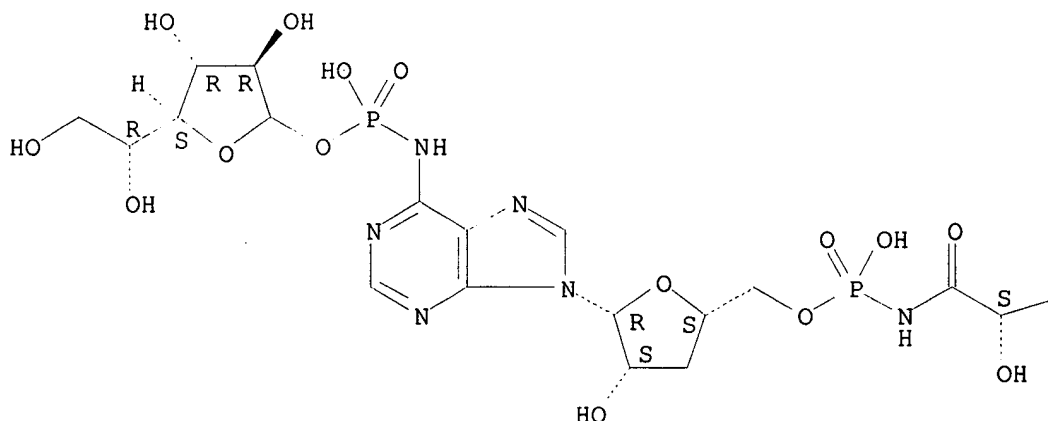
(sensitivity region for, of Ti plasmid, spontaneous insertion in)

RN 59111-78-3 HCAPLUS

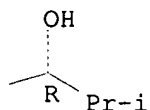
CN D-Glucofuranose, 1-[hydrogen [9-[3-deoxy-5-O-[[(4,5-dideoxy-4-methyl-D-threo-pentonoyl)amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



L7 ANSWER 47 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1986:436434 Document No. 105:36434 Modification of T-DNA of nopaline Ti plasmid by intermediary vector and utilization of agrocin 84 sensitivity as simple criterion of conjugation transfer of modified Ti plasmid.

Vlasak, J.; Hroudá, M.; Bisková, R.; Ondřej, M. (Inst. Exp. Bot., Czech. Acad. Sci., Ceske Budejovice, 370 05, Czech.). Folia Microbiol. (Prague), 31(2), 86-93 (English) 1986. CODEN: FOMIAZ. ISSN: 0015-5632.

AB The chloramphenicol-resistance gene from pSa was introduced into the T-DNA of pTi T37 of *Agrobacterium tumefaciens* by cointegration with an intermediary plasmid based on pBR322. The resulting intermediary vector

Searched by: Mary Hale 308-4258 CM-1 1E01

was mobilized to *A. tumefaciens* T37 by the conjugative plasmid pRK2. The RK2 plasmid also forms contegrates with pTi due to the Tn3 transposon which was used for the mobilization of modified pTi into a plasmid-less *A. tumefaciens* strain. Transconjugants were selected on the basis of their antibiotic-resistance markers and tested for agrocin sensitivity as proof of Ti plasmid transfer. Agrocin sensitivity of transconjugants together with chloramphenicol resistance was a sufficient and simple criterion of transfer of modified Ti plasmids. *Agrobacterium* Strains with modified Ti plasmids showed decreased virulence because of the presence of an addnl. borderline sequence inside their T-DNA.

IT 59111-78-3

RL: PRP (Properties)

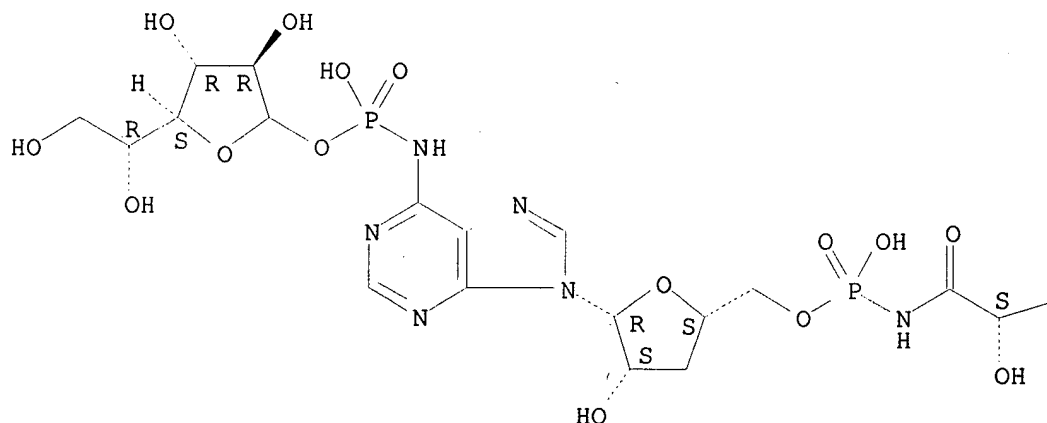
(sensitivity to, as criterion for conjugation transfer of Ti plasmid)

RN 59111-78-3 HCAPLUS

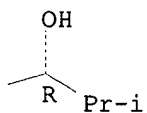
CN D-Glucofuranose, 1-[hydrogen [9-[3-deoxy-5-O-[[[(4,5-dideoxy-4-methyl-D-threo-pentonoyl)amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



L7 ANSWER 48 OF 77 HCAPLUS COPYRIGHT 2002 ACS
 1986:124823 Document No. 104:124823 Agrocin and the biological control of crown gall. Kerr, A.; Tate, M. E. (Waite Agric. Res. Inst., Univ. Adelaide, Glen Osmond, 5064, Australia). Microbiol. Sci., 1(1), 1-4 (English) 1984. CODEN: MISCEI. ISSN: 0265-1351.

Searched by: Mary Hale 308-4258 CM-1 1E01

AB A review with 23 refs. of agrocin, e.g., Agrocin 84 (I) [59111-78-3], Agrocin 108 [101026-84-0], and their effect for the control of crown gall. Genetics of I prodn. and other agrocin are discussed.

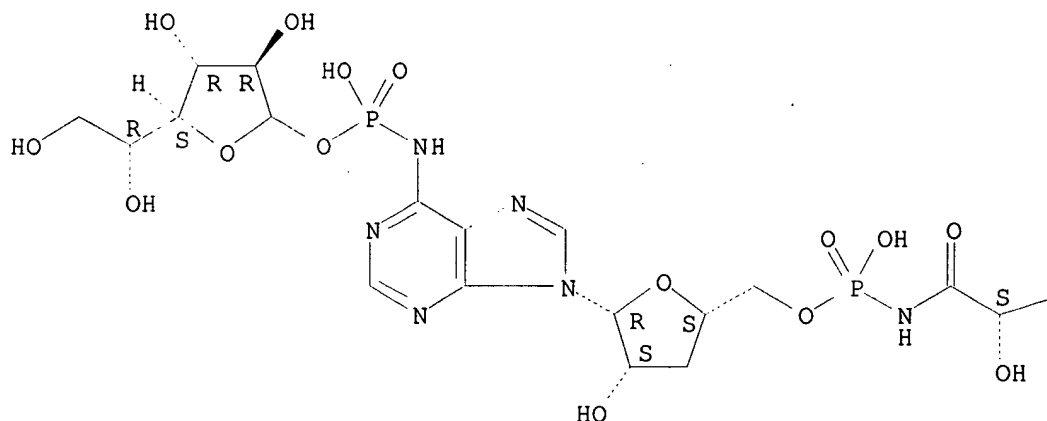
IT 59111-78-3
RL: BIOL (Biological study)
(crown gall control by)

RN 59111-78-3 HCAPLUS

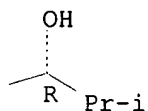
CN D-Glucofuranose, 1-[hydrogen [9-[3-deoxy-5-O-[[[4,5-dideoxy-4-methyl-D-threo-pentono-yl)amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



L7 ANSWER 49 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1985:417535 Document No. 103:17535 Tn5 insertions in the agrocin 84 plasmid: the conjugal nature of pAgK84 and the locations of determinants for transfer and agrocin 84 production. Farrand, Stephen K.; Slota, John E.; Shim, J. S.; Kerr, Allen (Stritch Sch. Med., Loyola Univ. Chicago, Maywood, IL, 60153, USA). Plasmid, 13(2), 106-17 (English) 1985. CODEN: PLSMDX. ISSN: 0147-619X.

AB The kanamycin-resistance transposon Tn5 was randomly introduced into pAgK84, a 47.7-kilobase (kb) plasmid coding for agrocin 84 [59111-78-3] prodn. in Agrobacterium. Using such marked plasmids, pAgK84 was found to be conjugal. It could be transferred to several

Searched by: Mary Hale 308-4258 CM-1 1E01

Agrobacterium strains including those harboring octopine- or nopaline-type Ti plasmids. Its presence has no effect on Ti plasmid functions such as opine utilization and tumorigenicity, but it does confer agrocin 84 immunity upon previously sensitive strains. The plasmid could also be conjugally transferred to a Nod+ Fix+ strain of Rhizobium meliloti. The prodn. of agrocin 84 is expressed in all Agrobacterium and Rhizobium transconjugants tested. The agrocin plasmid could not be introduced into restrictionless Escherichia coli or Pseudomonas aeruginosa recipients by conjugation or transformation. The sites of 92 independent Tn5 insertions were mapped on pAgK84. These insertions are dispersed over the entire length of the plasmid. Anal. of the sites and effects of the Tn5 insertions allowed construction of a functional map of pAgK84. Forty-three of these insertions, spanning a 20-kb segment of the plasmid, abolished or greatly reduced the prodn. of agrocin 84. The presence of 2 insertions within this segment having an effect on agrocin prodn. suggests that .gtoreq.3 regions of the plasmid are involved in agrocin 84 biosynthesis. Fourteen of the Tn5 insertion derivs. are no longer conjugally transferable. These insertions all map to a single region of the plasmid and define about 3.5-kb as being assocd. with transfer functions.

IT 59111-78-3

RL: PRP (Properties)

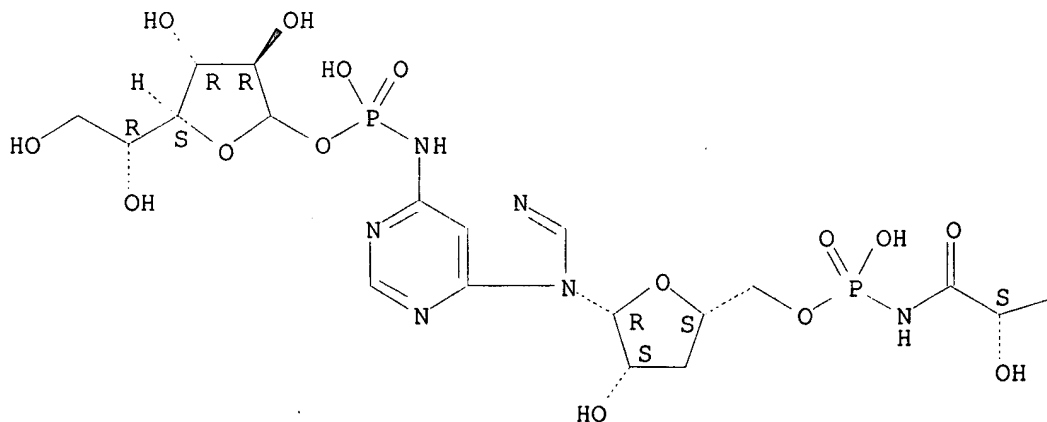
(genes for, of plasmid pAgK84, characterization and mapping of)

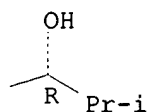
RN 59111-78-3 HCAPLUS

CN D-Glucofuranose, 1-[hydrogen [9-[3-deoxy-5-O-[[(4,5-dideoxy-4-methyl-D-threo-pentonoyl)amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A





L7 ANSWER 50 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1983:1075 Document No. 98:1075 Genetic isolation and physical characterization of pAgK84, the plasmid responsible for agrocin 84 production. Slota, John E.; Farrand, Stephen K. (Stritch Sch. Med., Loyola Univ. Chicago, Maywood, IL, 60153, USA). Plasmid, 8(2), 175-86 (English) 1982. CODEN: PLSMDX. ISSN: 0147-619X.

AB The plasmid responsible for agrocin 84 [59111-78-3] biosynthesis by Agrobacterium radiobacter strain K84 was genetically isolated, free from any opine-catabolic plasmids. This was accomplished by mobilizing the agrocin plasmid (pAgK84) into the Ti plasmid-free A. tumefaciens strain A136. The mobilizing element, pAt84a, was then cured from such a transconjugant by cultivation at 37.degree.. Derivs. of strain A136 harboring both plasmids, or pAgK84 alone, produce agrocin 84. The agrocin plasmid isolated from these strains is indistinguishable by restriction endonuclease anal. from that in strain K84. A phys. map of pAgK84 was constructed with respect to 6 restriction endonucleases. The plasmid is cut only once by XbaI and twice by HpaI. Hybridization anal. shows that pAgK84 is closely related to pAtBo542a, a 25-megadalton plamid from a virulent, agrocinogenic A. tumefaciens strain of European origin. However, pAgK84 shows no detectable homol. to octopine or nopaline-type Agrobacterium plasmids.

IT 59111-78-3

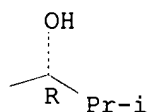
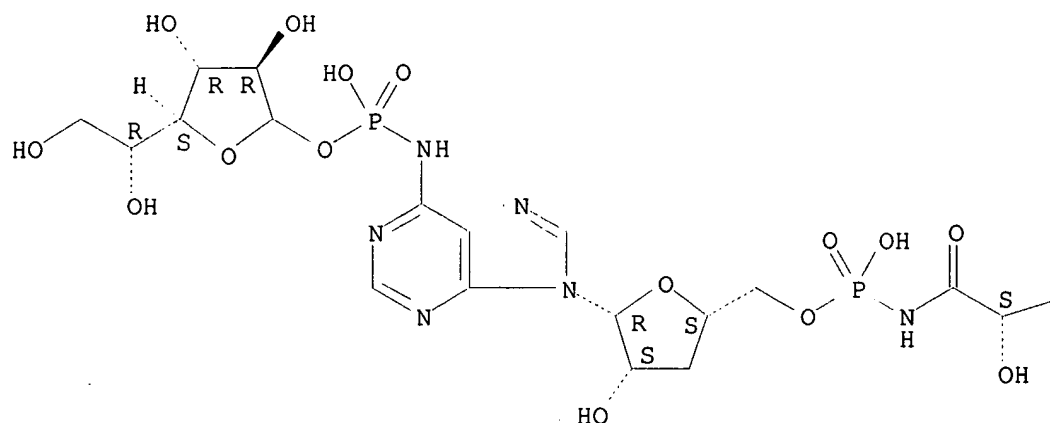
RL: FORM (Formation, nonpreparative)

(formation of, plasmid pAgK84-encoded, by Agrobacterium radiobacter)

RN 59111-78-3 HCAPLUS

CN D-Glucofuranose, 1-[hydrogen [9-[3-deoxy-5-O-[[[4,5-dideoxy-4-methyl-D-threo-pentonoyl)amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 51 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1982:612185 Document No. 97:212185 Biochemical studies on cytoplasmic membranes of agrocin sensitive and resistant strains of *Agrobacterium tumefaciens*. Basu, Mitali; Banerjee, Debabrata; Tewari, Raj; Das, Pijush K.; Chatterjee, Gora Chand (Dep. Biochem., Univ. Calcutta, Calcutta, 700 019, India). *Acta Microbiol. Pol.*, 31(1), 37-49 (English) 1982. CODEN: AMPOAX. ISSN: 0001-6195.

AB The cytoplasmic membrane of *A. tumefaciens* accounted for 12-13% of the dry wt. of the whole cells and consisted of 71% protein, 24% lipid (of which 70% was phospholipid), and 5-6% carbohydrates. The isolated cell membrane of *A. tumefaciens* was resolved into 15 carbohydrates. The cytoplasmic membranes of the virulent agrocin 84 (I)-sensitive and avirulent I-resistant strains of *A. tumefaciens* showed only minor quant. variation of the protein bands in gel electropherograms. The membrane proteins of these strains were antigenically identical, as studied by immunodiffusion and immunoelectrophoresis, and they cross-reacted with one another. The total lipid content of the membrane of I-resistant strains was higher than that of the normal strain. No appreciable differences were detected in the phospholipids, neutral lipids, or fatty acids of the whole cell and cytoplasmic membrane or among the cytoplasmic membrane fragments of the 3 strains studies.

IT 59111-78-3

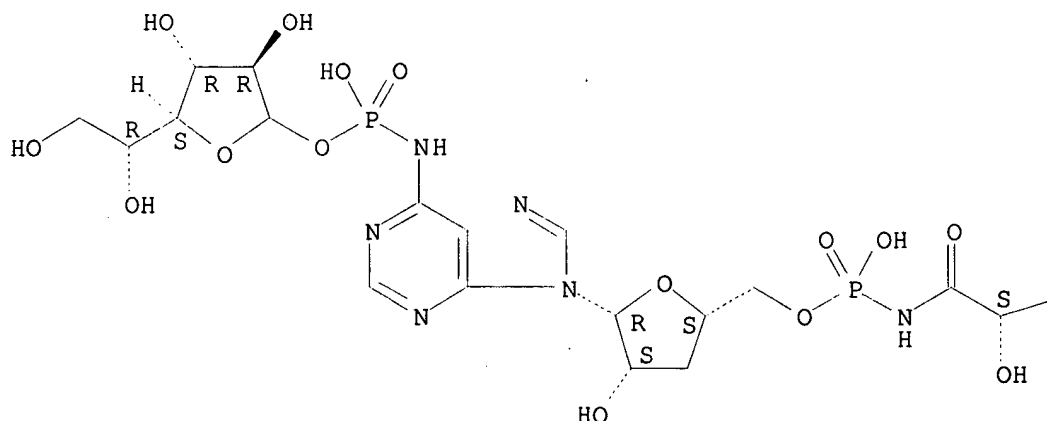
RL: BIOL (Biological study)

(resistance to, in *Agrobacterium tumefaciens*, cytoplasmic membrane

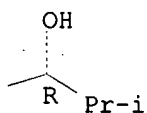
compn. in relation to)
 • RN 59111-78-3 HCAPLUS
 CN D-Glucofuranose, 1-[hydrogen [9-[3-deoxy-5-O-[[[4,5-dideoxy-4-methyl-D-threo-pentonoyl)amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

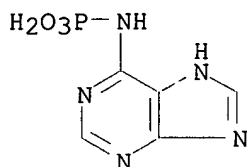


PAGE 1-B



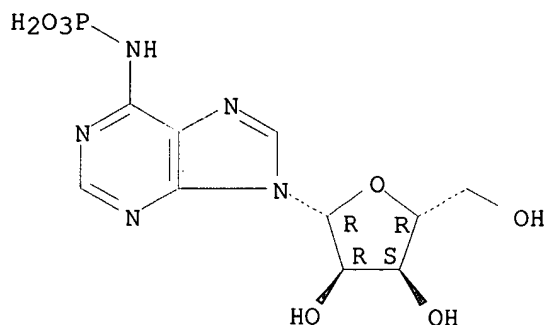
L7 ANSWER 52 OF 77 HCAPLUS COPYRIGHT 2002 ACS
 1982:558438 Document No. 97:158438 Physicochemical studies on phosphorylation. Ghosh, Guru Prasanna (Sheila Dhar Inst. Soil Sci., Allahabad Univ., Allahabad, 211 002, India). J. Indian Chem. Soc., 59(4), 599-602 (English) 1982. CODEN: JICSAH. ISSN: 0019-4522.
 AB Cryoscopic, ebullioscopic, conductometric, and pH detns. were carried out of orthophosphoric acid alone and mixed with adenine, creatine, glycine, asparagine, methionine, glutamic acid, urea, glucose, and sucrose. The results indicate that monomol. complexes are formed by the interaction of phosphoric acid with purines, creatine, and amino acids in the absence of enzymes and that these complexes are stable, even in boiling soln.
 IT **83305-93-5P 83305-95-7P**
 RL: PRP (Properties); PREP (Preparation)
 (formation and stability const. of)
 RN 83305-93-5 HCAPLUS
 CN Phosphoramidic acid, 1H-purin-6-yl- (9CI) (CA INDEX NAME)

Searched by: Mary Hale 308-4258 CM-1 1E01



RN 83305-95-7 HCAPLUS
 CN Phosphoramidic acid, (9-.beta.-D-ribofuranosyl-9H-purin-6-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 53 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1982:506913 Document No. 97:106913 Biological control of crown gall with an agrocin mutant of *Agrobacterium radiobacter*. Cooksey, D. A.; Moore, L. W. (Dep. Bot. Plant Pathol., Oregon State Univ., Corvallis, OR, 97331, USA). *Phytopathology*, 72(7), 919-21 (English) 1982. CODEN: PHYTAJ. ISSN: 0031-949X.

AB A mutant of *A. radiobacter* K84 that no longer produced agrocin 84 was obtained by mitomycin C curing of the 30-megadalton (Md) bacteriocinogenic plamid in K84. This mutant (designated K84 Arg-) no longer prevented crown gall of tomato stems when coinoculated with an agrocin-sensitive pathogen *A. tumefaciens* K24. However, it effectively reduced infection when it was placed on the host plant 24 h before the pathogen. In addn., either K84 or K84Agr- reduced infection by agrocin-resistant *A. tumefaciens* B6 when the antagonists were applied 24 h before the pathogen. Tumor wts. were reduced when K84 Agr- was coinoculated with K24 or B6, or when it was applied 24 h before the pathogens. Apparently, other mechanisms, such as phys. blockage of infection sites, are involved in biol. control by K84 in addn. to prodn. of agrocin 84.

IT 59111-78-3

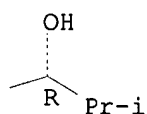
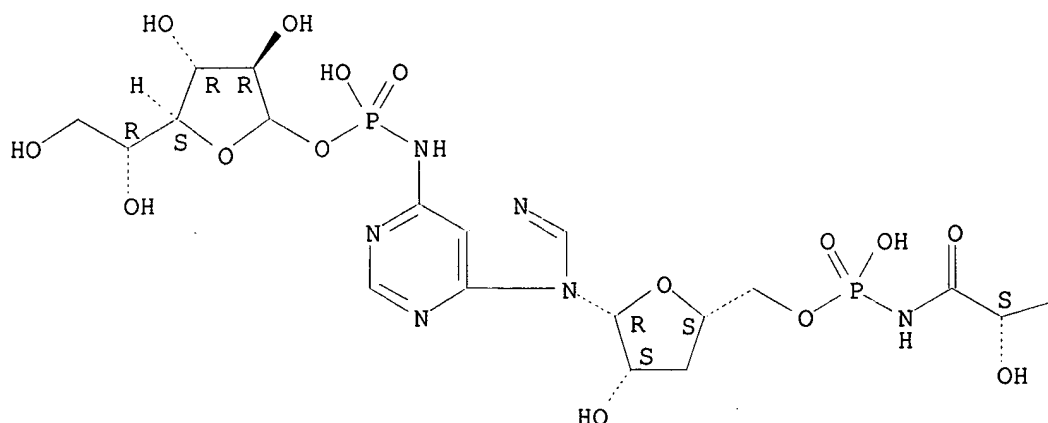
RL: BIOL (Biological study)

(*Agrobacterium radiobacter* mutant deficient in, crown gall control by)

RN 59111-78-3 HCAPLUS

CN D-Glucofuranose, 1-[hydrogen [9-[3-deoxy-5-O-[[[(4,5-dideoxy-4-methyl-D-threo-pentonoyl)amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

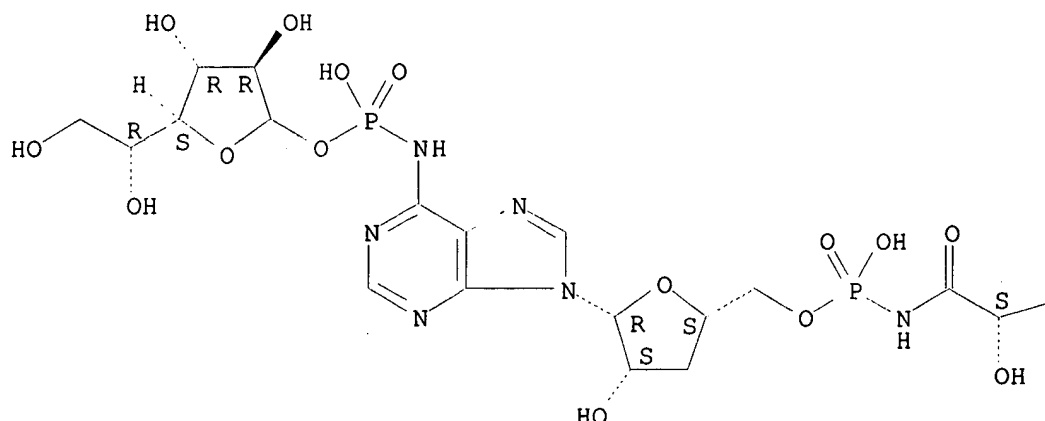
Absolute stereochemistry.



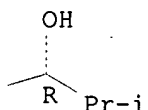
- L7 ANSWER 54 OF 77 HCAPLUS COPYRIGHT 2002 ACS
 1982:506845 Document No. 97:106845 Isolation and properties of transfer regulatory mutants of the nopaline Ti-plasmid pTiC58. Ellis, J. G.; Murphy, P. J.; Kerr, A. (Dep. Plant Pathol., Waite Agric. Res. Inst., Glen Osmond, 5064, Australia). MGG, Mol. Gen. Genet., 186(2), 275-81 (English) 1982. CODEN: MGGEAE. ISSN: 0026-8925.
- AB Conjugal transfer of the nopaline Ti-plasmid pTiC58 is inducible in *Agrobacterium tumefaciens* by the phosphorylated opines, agrocinopines A and B. Although the uninduced level of transfer is negligible (<10⁻⁷/donor), some transconjugants have been isolated from crosses performed in the absence of agrocinopine. These transconjugants harbor mutant Ti-plasmids that transfer constitutively (>10⁻³/donor). These mutants have several other correlated phenotypes including constitutive uptake of agrocinopine. These mutants also possess a supersensitivity to agrocin 84 and the ability to prevent the excretion of agrocin 84 when they are present in the same cell as the agrocin 84 biosynthetic plasmid pAt-84a.
- IT **59111-78-3**
 RL: PROC (Process)
 (transport of, by *Agrobacterium tumefaciens*, plasmid pTiC58 in)
- RN 59111-78-3 HCAPLUS
- CN D-Glucofuranose, 1-[hydrogen [9-[3-deoxy-5-O-[[[4,5-dideoxy-4-methyl-D-threo-pentonoyl)amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



- L7 ANSWER 55 OF 77 HCAPLUS COPYRIGHT 2002 ACS
1982:504845 Document No. 97:104845 Characteristics of Ti plasmids from broad-host-range and ecologically specific biotype 2 and 3 strains of *Agrobacterium tumefaciens*. Perry, Keith L.; Kado, Clarence I. (Dep. Plant Pathol., Univ. California, Davis, CA, 95616, USA). *J. Bacteriol.*, 151(1), 343-50 (English) 1982. CODEN: JOBAAY. ISSN: 0021-9193.
- AB *A. tumefaciens* Strains isolated from crown gall tumors on grapevines in California were consistently of the biotype 3 group. All 11 of these strains were limited in their host range and harbored Ti plasmids with mol. masses of 119-142 megadaltons (Mdal) as well as a larger cryptic plasmid of >200 Mdal; occasionally a smaller cryptic plasmid of 65 Mdal was also present. Ti plasmids of these strains have DNA sequences in common with Ti plasmids of octopine [34522-32-2] and nopaline [22350-70-5] strains belonging to the biotype 1 group and exhibited sequence homologies with the conserved region of the T-DNA. Ten of the 11 strains utilized octopine as a sole source of C and N, and 3 strains catabolized both octopine and nopaline, whereas 1 strain catabolized only nopaline. All of these strains were resistant to the bacteriocin agrocin-84 [59111-78-3], except 1 grapevine strain that belonged to the biotype 1 group and was agrocin sensitive; it also differed in its plasmid and virulence characteristics. Isolations from *Rubus ursinus* ollalieber berry galls yielded exclusively biotype 2 strains.

These strains were insensitive to agrocin-84, utilized nopaline as a sole C and N source, and were highly virulent on all host plants tested. They contained Ti plasmids of 100-130 Mdal and occasionally a cryptic plasmid of 69 Mdal. Their Ti plasmids have DNA sequences in common with Ti plasmids of biotype 1 strains and with the conserved region of the T-DNA.

IT 59111-78-3

RL: PRP (Properties)

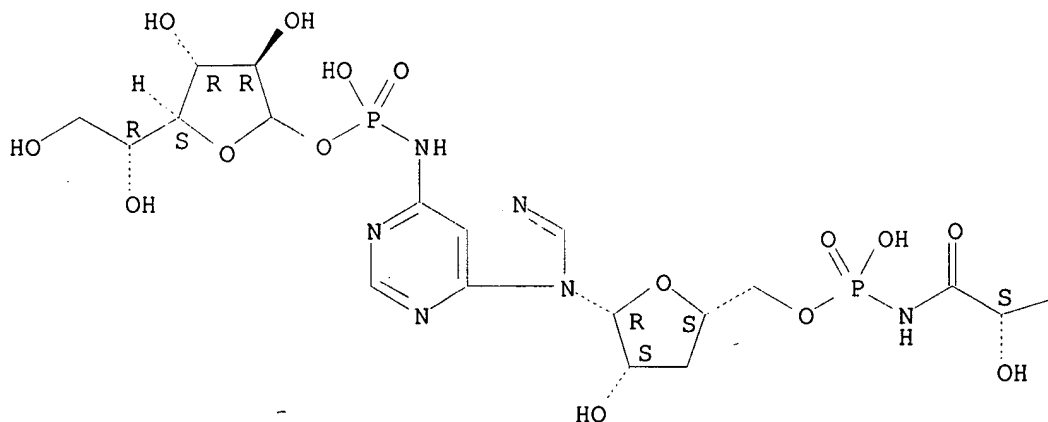
(resistance to, of *Agrobacterium tumefaciens*, plasmid Ti homol. in relation to)

RN 59111-78-3 HCAPLUS

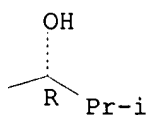
CN D-Glucofuranose, 1-[hydrogen [9-[3-deoxy-5-O-[[[(4,5-dideoxy-4-methyl-D-threo-pentono-1-yl)amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



L7 ANSWER 56 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1982:214695 Document No. 96:214695 Vasoactivities of adenosine analogs in trout gill (*Salmo gairdneri* R.). Colin, Didier A.; Leray, Claude (Lab. Physiol. Comp. Regul., CNRS, Strasbourg, F-67037, Fr.). Biochem. Pharmacol., 30(21), 2971-7 (English) 1981. CODEN: BCPA6. ISSN: 0006-2952.

AB Various adenosine analogs, phosphorylated or not, modified at the purine or in the carbohydrate moiety, were tested for their ability to induce a vasoconstriction in the arterio-arterial vascular bed of the trout gill.

Searched by: Mary Hale 308-4258 CM-1 1E01

Structure-activity relations were detd. The results sustained the hypothesis of the presence of specific vascular purinergic receptors in the trout gill.

IT 78098-66-5 78111-41-8

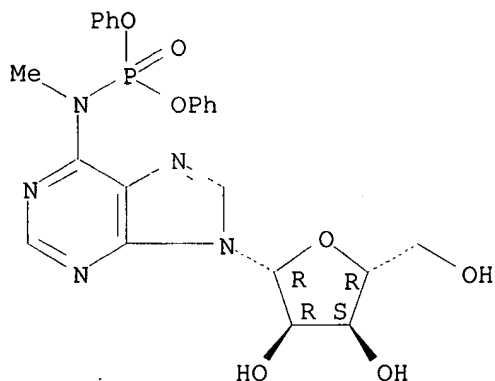
RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)

(artery constriction by, in gill of trout, purine receptors in relation to)

RN 78098-66-5 HCAPLUS

CN Phosphoramidic acid, methyl(9-.beta.-D-ribofuranosyl-9H-purin-6-yl)-, diphenyl ester (9CI) (CA INDEX NAME)

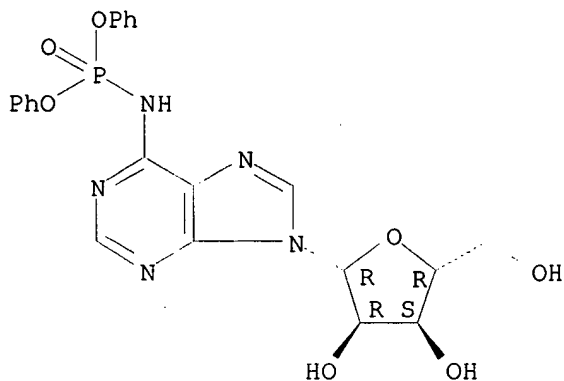
Absolute stereochemistry.



RN 78111-41-8 HCAPLUS

CN Adenosine, N-(diphenoxyphosphinyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 57 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1981:493214 Document No. 95:93214 Determination of ionization constants by paper electrophoresis. Tate, Max E. (Dep. Agric. Biochem., Univ. Adelaide, Glen Osmond, 5064, Australia). Biochem. J., 195(2), 419-26 (English) 1981. CODEN: BIJOAK. ISSN: 0306-3275.

AB Dimensionless apparent ionization consts. of charged low-mol.-wt. species were obtained from paper-electrophoretic data at 20-5.degree. with buffers (I 0.1-0.5) of measured pH (1.5-12.5) contg. oxalate ions. Relative, rather than abs., mobilities were measured by using glycerol and m-nitrobenzenesulfonate resp. as stds. of zero and unit mobility.

Searched by: Mary Hale 308-4258 CM-1 1E01

Application of the procedure to ionizations of adenine, adenosine, 2'-deoxyadenosine, 3'-deoxyadenosine, cAMP, ADP, ADP-glucose, agrocin 84, and ATP is described.

IT 59111-78-3

RL: PRP (Properties)

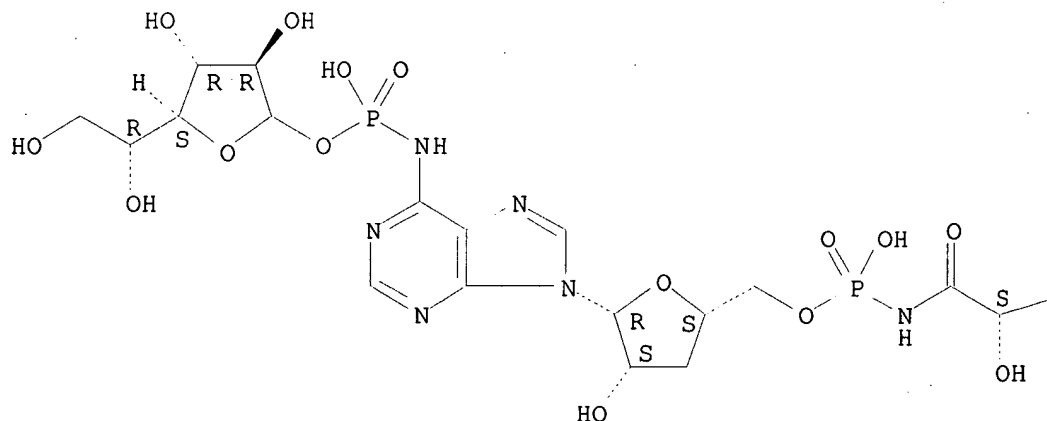
(ionization const. of, detn. of, by paper electrophoresis)

RN 59111-78-3 HCAPLUS

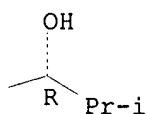
CN D-Glucofuranose, 1-[hydrogen [9-[3-deoxy-5-O-[[(4,5-dideoxy-4-methyl-D-threo-pentonoyl)amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



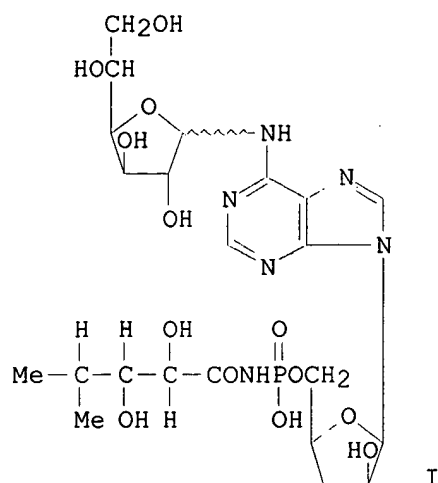
PAGE 1-B



L7 ANSWER 58 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1981:436238 Document No. 95:36238 Substituents at N6 and C-5' control selective uptake and toxicity of the adenine-nucleotide bacteriocin, agrocin 84, in agrobacteria. Murphy, Peter J.; Tate, Max E.; Kerr, Allen (Waite Agric. Res. Inst., Univ. Adelaide, Adelaide, 5064, Australia). Eur. J. Biochem., 115(3), 539-43 (English) 1981. CODEN: EJBCAI. ISSN: 0014-2956.

GI



AB The inhibition of a sensitive strain of *Agrobacterium radiobacter* by the nucleotide bacteriocin agrocin 84 (I) [59111-78-3] was detd., and a structure-function study of the I mol. was undertaken. Two I nucleotide fragments lacking either the N6 [77822-25-4] or 5'-phosphoramidate [72666-23-0] substituents were used in uptake studies of [^{32}P]I, establishing that the plasmid-controlled, strain-specific uptake of I is detd. by the N6-D-glucofuranosyloxyposphoramidate substituent. This was further supported by the markedly reduced uptake of the ^{32}P -labeled fragment lacking the N6-substituent. Equil. dialysis studies indicated that the N6-substituent is recognized by a binding protein involved in the uptake of I into sensitive strains. The nucleotide fragment bearing the N6-substituent was a competitive inhibitor for the uptake of I in vivo with a $K_i = 1.0 \times 10^{-7}\text{M}$ and was itself selectively transported into a sensitive strain at a rate comparable with I; unlike I however, it is nontoxic. By contrast, the fragment bearing the 5'-phosphoramidate was taken up by both sensitive and insensitive strains at a barely measurable rate and was toxic to both.

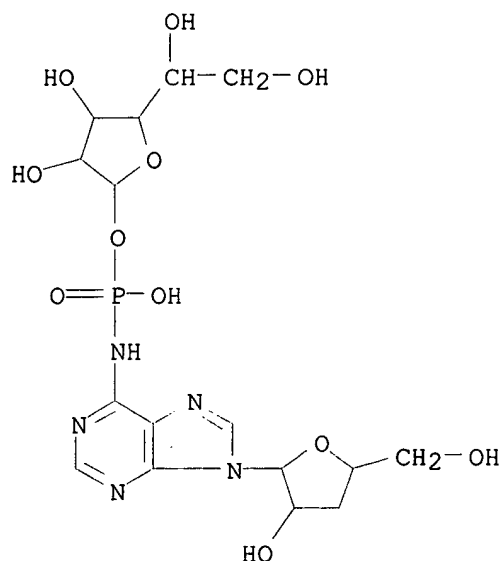
IT 72666-23-0

RL: PRP (Properties)

(agrocin 84 uptake by *Agrobacterium radiobacter* inhibition by)

RN 72666-23-0 HCAPLUS

CN D-Glucofuranose, 1-[hydrogen [9-(3-deoxy-.beta.-D-threo-pentofuranosyl)-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)



IT 59111-78-3

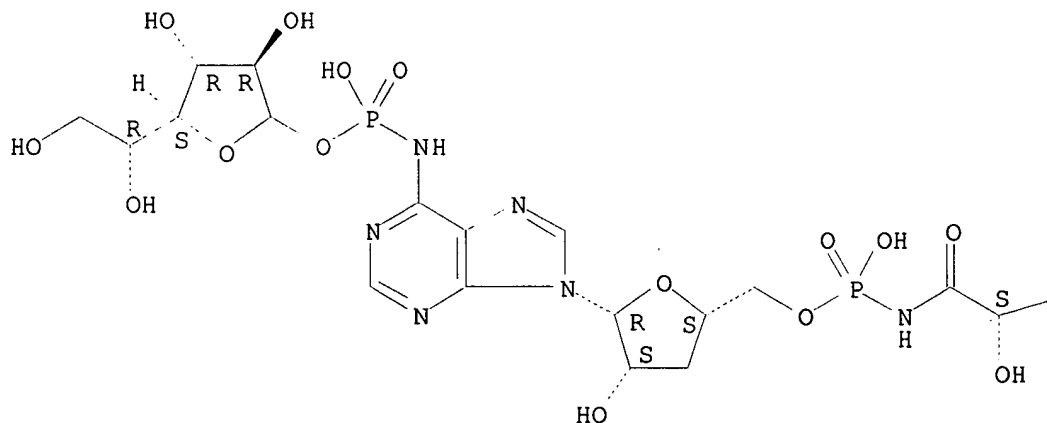
RL: BPR (Biological process); BIOL (Biological study); PROC (Process)
(metab. of, by Agrobacterium radiobacter, bactericidal activity in
relation to)

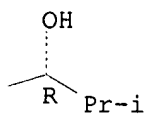
RN 59111-78-3 HCAPLUS

CN D-Glucofuranose, 1-[hydrogen [9-[3-deoxy-5-O-[[(4,5-dideoxy-4-methyl-D-
threo-pentonoyl)amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-
purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A





L7 ANSWER 59 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1981:425488 Document No. 95:25488 Nucleotides. XIII. Phosphorylations of adenosine and 2'-deoxyadenosine by phosphorochloridates. Charubala, Ramamurthy; Pfleiderer, Wolfgang (Fak. Chem., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger.). Heterocycles, 15(2), 761-76 (English) 1981. CODEN: HTCYAM. ISSN: 0385-5414.

AB Phosphorylations of adenosine and 2'-deoxyadenosine by various phosphorylating agents, e.g., (PhO)₂P(O)Cl, were achieved at positions 3', 5', and N-6 using appropriate starting materials for unambiguous synthesis. There is a difference in the reactivity of the different functions in these mols. with a preference of the 5'-OH followed by 6-NH₂ and then 3'-OH in the 3rd place. UV and CD spectral data and pK_a values of various adenosine and 2'-deoxyadenosine phosphotriesters prep'd. are given.

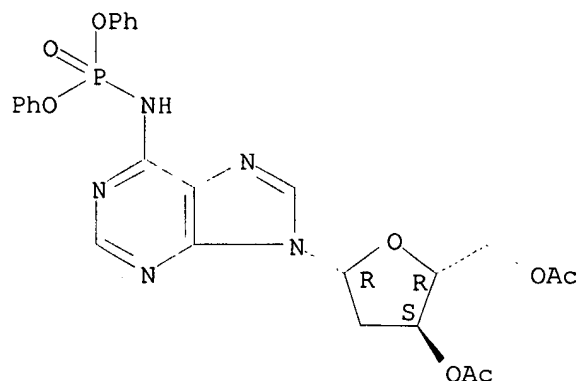
IT 78098-63-2P 78098-64-3P 78098-65-4P
78098-67-6P 78098-68-7P 78098-69-8P
78098-70-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and deacetylation of)

RN 78098-63-2 HCAPLUS

CN Phosphoramidic acid, [9-(3,5-di-O-acetyl-2-deoxy-.beta.-D-erythro-pentofuranosyl)-9H-purin-6-yl]-, diphenyl ester (9CI) (CA INDEX NAME)

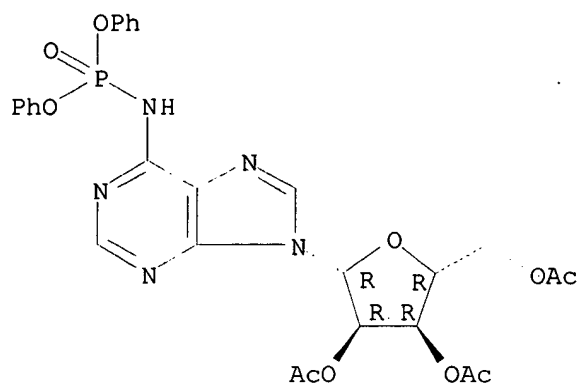
Absolute stereochemistry.



RN 78098-64-3 HCAPLUS

CN Phosphoramidic acid, [9-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, diphenyl ester (9CI) (CA INDEX NAME)

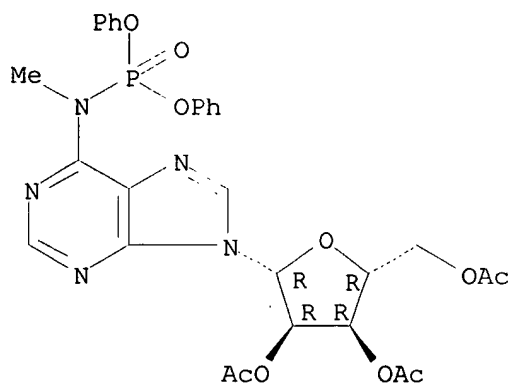
Absolute stereochemistry.



RN 78098-65-4 HCAPLUS

CN Phosphoramidic acid, methyl[9-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, diphenyl ester (9CI) (CA INDEX NAME)

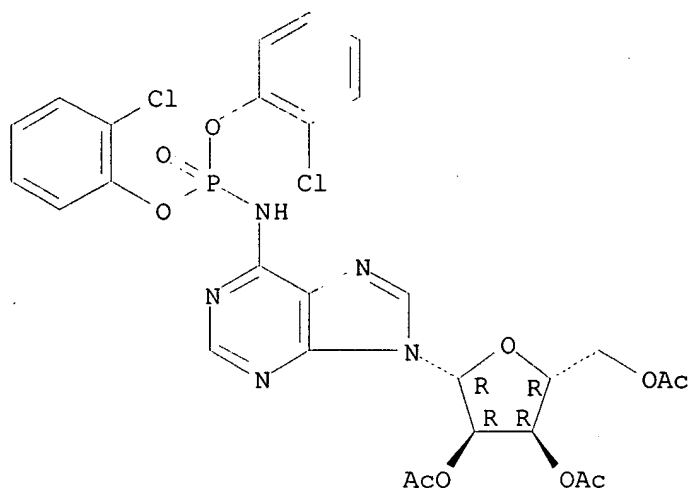
Absolute stereochemistry.



RN 78098-67-6 HCAPLUS

CN Phosphoramidic acid, [9-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, bis(2-chlorophenyl) ester (9CI) (CA INDEX NAME)

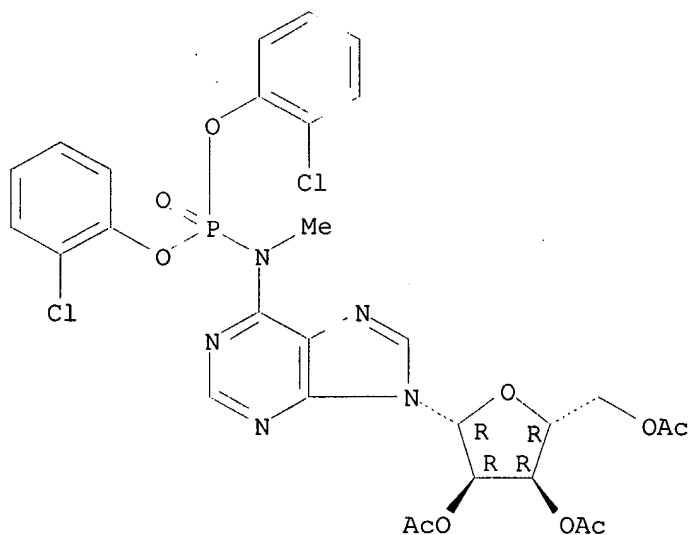
Absolute stereochemistry.



RN 78098-68-7 HCAPLUS

CN Phosphoramidic acid, methyl[9-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, bis(2-chlorophenyl) ester (9CI) (CA INDEX NAME)

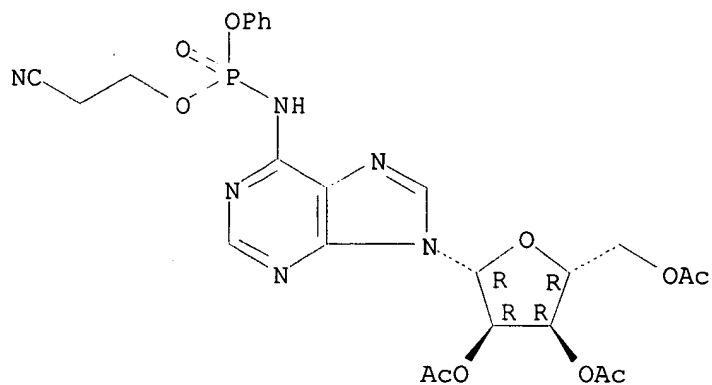
Absolute stereochemistry.



RN 78098-69-8 HCAPLUS

CN Phosphoramidic acid, [9-(2,3,5-tri-O-acetyl-.beta.-D-ribofuranosyl)-9H-purin-6-yl]-, 2-cyanoethyl phenyl ester (9CI) (CA INDEX NAME)

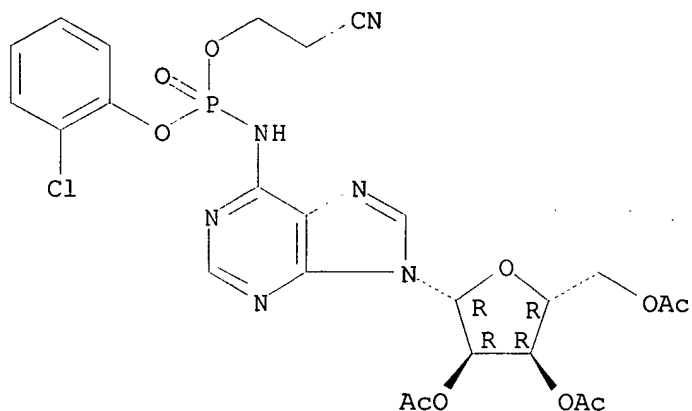
Absolute stereochemistry.



RN 78098-70-1 HCAPLUS

CN Phosphoramidic acid, [9-(2,3,5-tri-O-acetyl-beta-D-ribofuranosyl)-9H-purin-6-yl]-, 2-chlorophenyl 2-cyanoethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 78098-53-0P 78098-55-2P 78098-56-3P

78098-57-4P 78098-58-5P 78098-60-9P

78098-66-5P 78098-71-2P 78111-40-7P

78111-41-8P 78111-42-9P 78111-43-0P

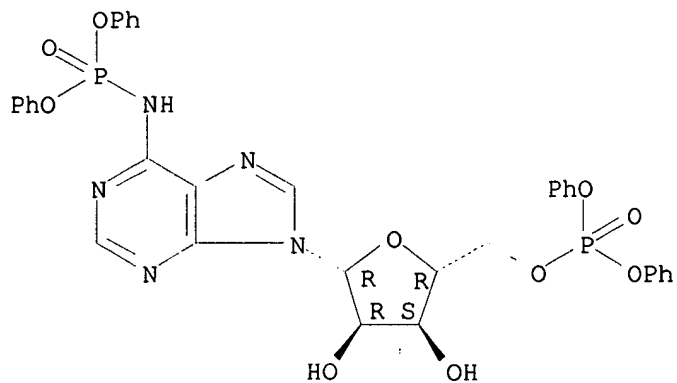
78111-44-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 78098-53-0 HCAPLUS

CN 5'-Adenylic acid, N-(diphenoxyphosphinyl)-, diphenyl ester (9CI) (CA INDEX NAME)

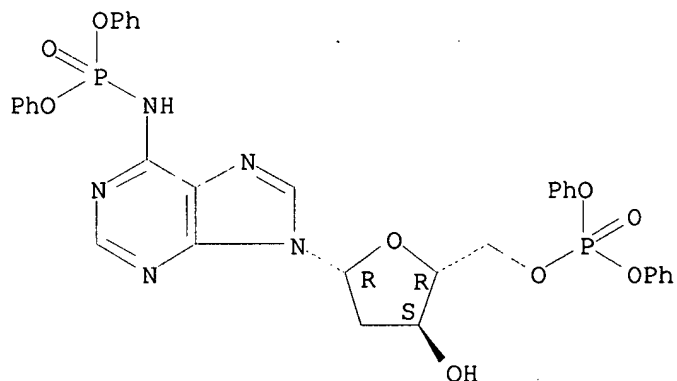
Absolute stereochemistry.



RN 78098-55-2 HCAPLUS

CN 5'-Adenylic acid, 2'-deoxy-N-(diphenoxyphosphinyl)-, diphenyl ester (9CI)
(CA INDEX NAME)

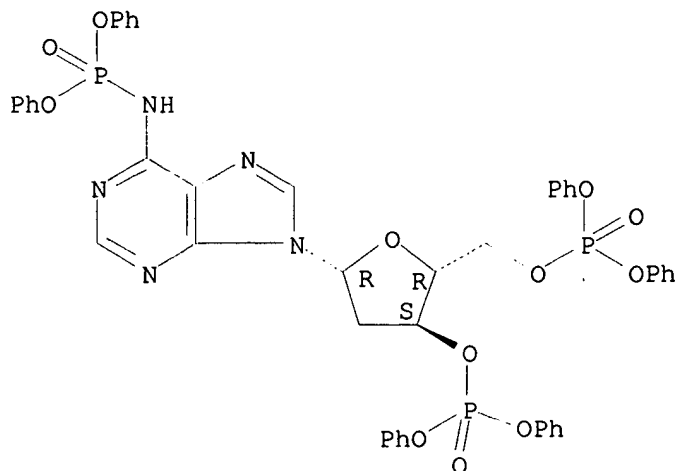
Absolute stereochemistry.



RN 78098-56-3 HCAPLUS

CN 3'-Adenylic acid, 2'-deoxy-N-(diphenoxyphosphinyl)-, diphenyl ester,
5'-(diphenyl phosphate) (9CI) (CA INDEX NAME)

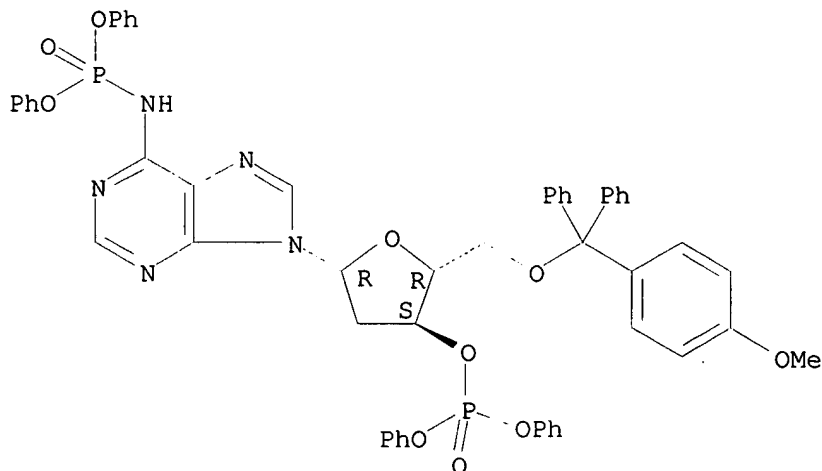
Absolute stereochemistry.



RN 78098-57-4 HCAPLUS

CN 3'-Adenylic acid, 2'-deoxy-N-(diphenoxyposphinyl)-5'-O-[(4-methoxyphenyl)diphenylmethyl]-, diphenyl ester (9CI) (CA INDEX NAME)

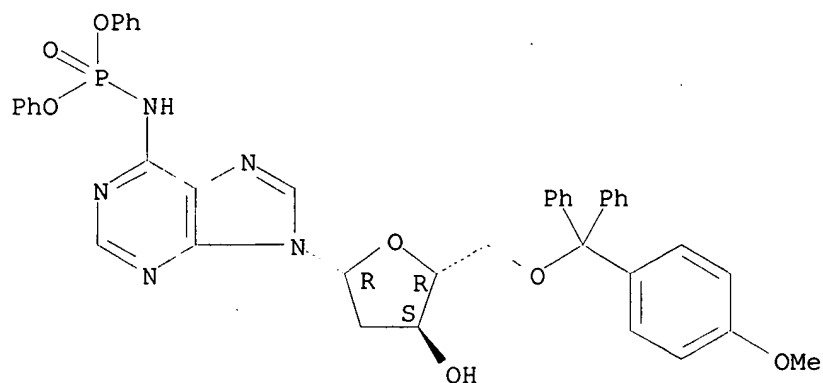
Absolute stereochemistry.



RN 78098-58-5 HCAPLUS

CN Phosphoramidic acid, [9-[2-deoxy-5-O-[(4-methoxyphenyl)diphenylmethyl]-.beta.-D-erythro-pentofuranosyl]-9H-purin-6-yl]-, diphenyl ester (9CI) (CA INDEX NAME)

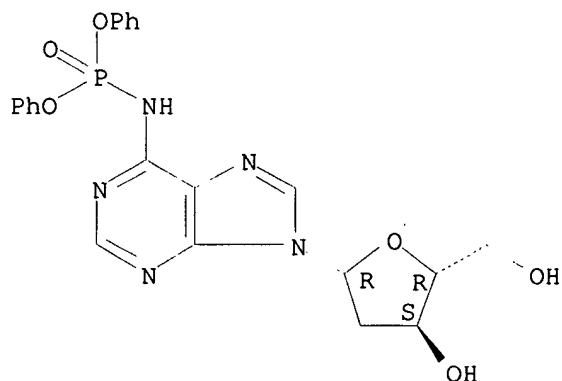
Absolute stereochemistry.



RN 78098-60-9 HCAPLUS

CN Phosphoramidic acid, [9-(2-deoxy-.beta.-D-erythro-pentofuranosyl)-9H-purin-6-yl]-, diphenyl ester (9CI) (CA INDEX NAME)

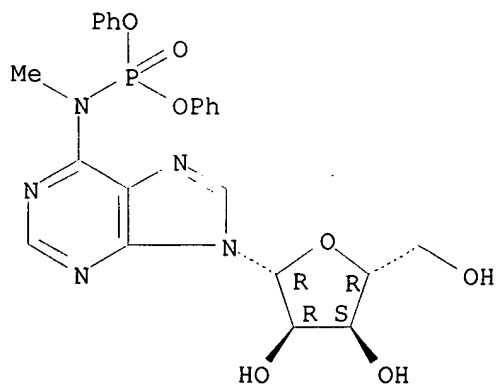
Absolute stereochemistry.



RN 78098-66-5 HCAPLUS

CN Phosphoramidic acid, methyl(9-.beta.-D-ribofuranosyl-9H-purin-6-yl)-, diphenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

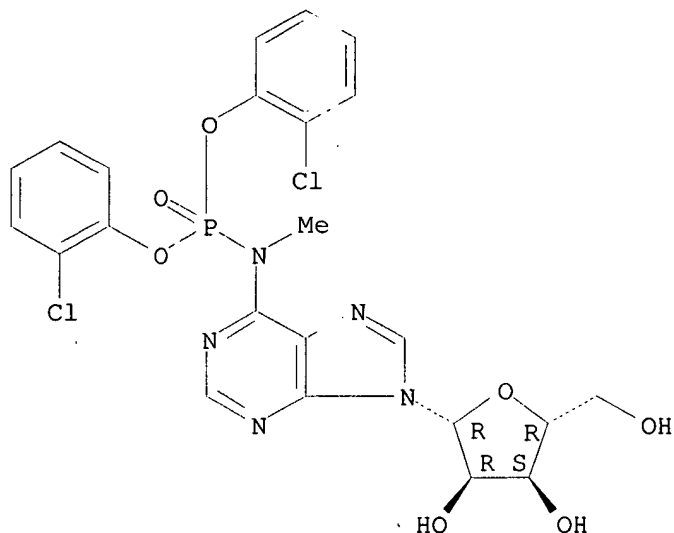


RN 78098-71-2 HCAPLUS

Searched by: Mary Hale 308-4258 CM-1 1E01

CN Phosphoramidic acid, methyl(9-.beta.-D-ribofuranosyl-9H-purin-6-yl)-, bis(2-chlorophenyl) ester (9CI) (CA INDEX NAME)

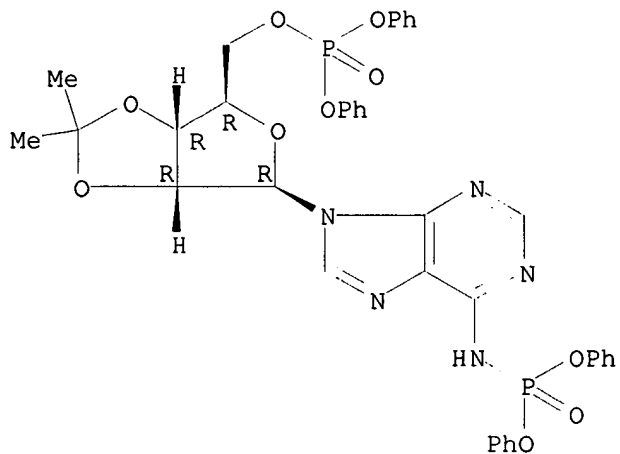
Absolute stereochemistry.



RN 78111-40-7 HCAPLUS

CN 5'-Adenylic acid, N-(diphenoxyphosphinyl)-2',3'-O-(1-methylethylidene)-, diphenyl ester (9CI) (CA INDEX NAME)

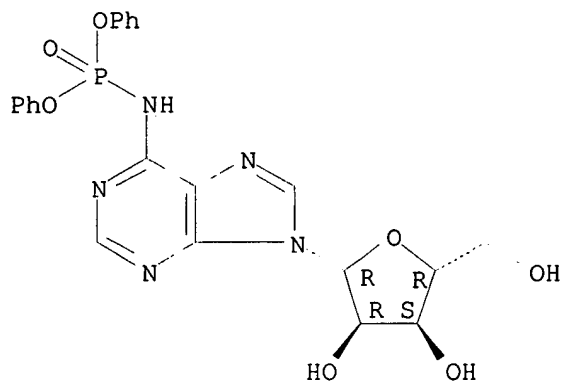
Absolute stereochemistry.



RN 78111-41-8 HCAPLUS

CN Adenosine, N-(diphenoxyphosphinyl)- (9CI) (CA INDEX NAME)

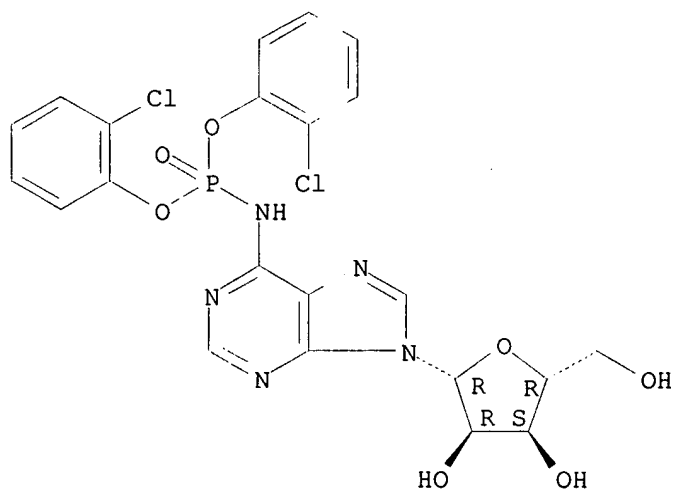
Absolute stereochemistry.



RN 78111-42-9 HCAPLUS

CN Adenosine, N-[bis(2-chlorophenoxy)phosphinyl]- (9CI) (CA INDEX NAME)

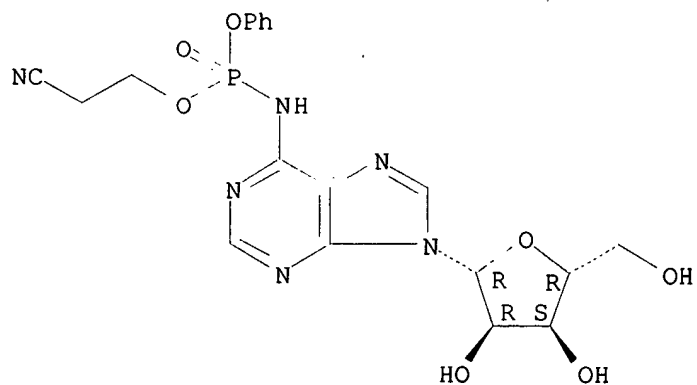
Absolute stereochemistry.



RN 78111-43-0 HCAPLUS

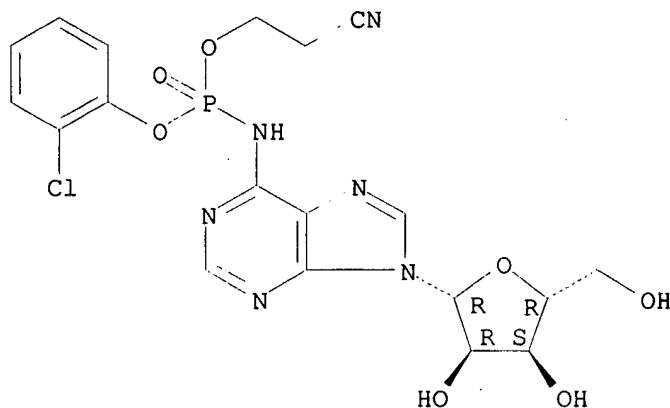
CN Adenosine, N-[(2-cyanoethoxy)phenoxyphosphinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



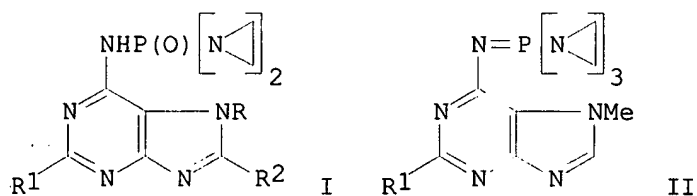
RN 78111-44-1 HCAPLUS
 CN Adenosine, N-[(2-chlorophenoxy)(2-cyanoethoxy)phosphinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 60 OF 77 HCAPLUS COPYRIGHT 2002 ACS
 1981:407223 Document No. 95:7223 Synthesis and antineoplastic activity of 6-diethylenimidophosphamido- and 6-triethyleniminophosphazopurines. Glushkov, R. G.; Nikolaeva, L. A.; Golovchinskaya, E. S.; Chernov, V. A.; Kravchenko, A. I.; Kozlova, O. V.; Gutorov, L. A. (Vses. Nauchno-Issled. Khim.-Farm. Inst., Moscow, USSR). Khim.-Farm. Zh., 15(3), 16-20 (Russian) 1981. CODEN: KHFZAN. ISSN: 0023-1134.

GI



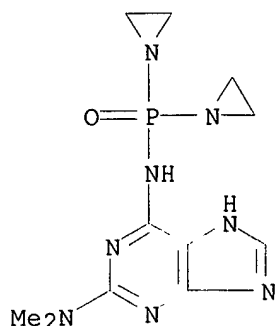
AB The title compds. I (R = Me, PhCH₂, H, R₁ = NMe₂, pyrrolidino, 2,2-dimethylpyrrolidino, piperidino, morpholino, R₂ = H, Cl, morpholino) and II (R₁ = NMe₂, pyrrolidino, 2,2-dimethylpyrrolidino) were obtained in 47.1-81.0% yields (I) and 48.7-61.3% yields (II) by phosphorylation of the amino group of a 6-aminopurine by POCl₃-aziridine and PCl₅-aziridine, resp. I and II were effective neoplasm inhibitors for Sarcoma 45 and Sarcoma 180 in white mice and rats.

IT 77931-46-5P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. and neoplasm-inhibiting activity of)

RN 77931-46-5 HCAPLUS

CN Phosphinic amide, P,P-bis(1-aziridinyl)-N-[2-(dimethylamino)-1H-purin-6-yl]- (9CI) (CA INDEX NAME)



L7 ANSWER 61 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1981:41972. Document No. 94:41972 Agrocin resistance in virulent derivatives of *Agrobacterium tumefaciens* harboring the pTi plasmid. Suele, S.; Kado, C. I. (Dep. Plant Pathol., Univ. California, Davis, CA, 95616, USA). *Physiol. Plant Pathol.*, 17(3), 347-56, 3 plates (English) 1980. CODEN: PPPYBC. ISSN: 0048-4059.

AB Exposure of *A. tumefaciens* strains C58 and O to purified agrocin 84 [59111-78-3] yields many mutants that are resistant to this bacteriocin and yet harbor the pTi plasmid and retain virulence. Among these mutants are those that are semiresistant, requiring higher doses of agrocin to show any degree of sensitivity. Like the totally resistant virulent mutants, these semiresistant mutants also retained higher virulence. Studies using [32P]agrocin clearly showed that agrocin-sensitive strains harboring the pTi plasmid readily take up agrocin whereas agrocin-resistant mutants, also harboring the pTi plasmid, take up negligible amts. of agrocin. Transfer of pTi plasmid from virulent agrocin-resistant mutants to an avirulent pTi plasmidless strain by genetic crosses in planta and in vitro continued to confer agrocin resistance and resistance to its uptake. On the other hand, pTi transferred from agrocin-sensitive strains conferred a high degree of sensitivity to the recipient and high levels of agrocin uptake. No differences in the pTi plasmids were obsd. between wild-type and agrocin-resistant mutants as judged by restriction endonuclease fragment analyses in agarose gel electrophoretograms. Agrocin-sensitive revertants were obtained from cloned resistant mutants. These revertants displayed partial sensitivity to agrocin only, suggesting that either point, small frameshift, or insertional mutations had taken place. The predominance of agrocin 84-resistant mutants harboring the pTi plasmid and retaining their virulence may complicate the current concepts concerning biol. control with agrocin 84-producing strains.

IT 59111-78-3

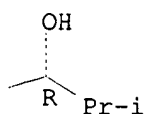
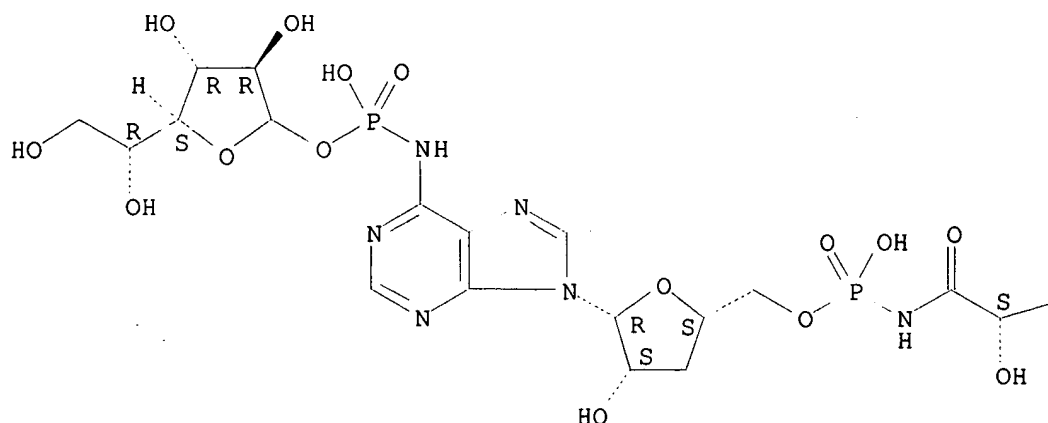
RL: PRP (Properties)

(*Agrobacterium tumefaciens* resistance to, plasmid pTi and virulence in relation to)

RN 59111-78-3 HCAPLUS

CN D-Glucofuranose, 1-[hydrogen [9-[3-deoxy-5-O-[[[(4,5-dideoxy-4-methyl-D-threo-pentono-yl)amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 62 OF 77 HCAPLUS COPYRIGHT 2002 ACS
 1980:472346 Document No. 93:72346 Functional monomers and polymers. 77.
 Synthesis and polymerization of acryloylamino derivatives of nucleic acid
 bases. Kondo, Koichi; Tanioku, Shozo; Takemoto, Kiichi (Fac. Eng., Osaka
 Univ., Suita, Japan). Makromol. Chem., Rapid Commun., 1(5), 303-6
 (English) 1980. CODEN: MCRCD4.

AB Purinylethylacrylamide derivs. and N-[4-(4-ethoxy-2-oxo-1,2-
 dihydropyrimidin-1-ylmethyl)phenyl]acrylamide [74242-05-0] (prepd. from
 acrylic anhydride and the appropriate amine) were subjected to H-transfer
 polymn. for 20 h at 100.degree. in DMF, DMSO, or pyridine, giving products
 with mol. wt. 2000 (MeOH-sol.) and 8000 (MeOH-insol.).

IT **74242-14-1P**
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and NMR of)

RN 74242-14-1 HCAPLUS

CN 2-Propenamide, N-[2-[6-[(diphenylphosphinothioyl)amino]-9H-purin-9-
 yl]ethyl]-, homopolymer (9CI) (CA INDEX NAME)

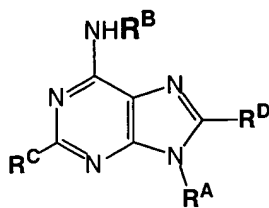
CM 1

CRN 74242-13-0

CMF C22 H21 N6 O P S

Claims

1. A compound of formula (I) (or a pharmaceutically acceptable derivative thereof):



(I)

wherein

R^A is hydrogen, or an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

R^B is an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety which comprises one or more phosphorus-containing moieties;

R^C is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or -ZR, wherein Z is -O-, -S-, or NR, wherein each occurrence of R without a further alphanumeric superscript is independently hydrogen, or a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

R^D is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or -ZR;

wherein in each of the foregoing groups each aliphatic or heteroaliphatic moiety may be branched or unbranched, cyclic or acyclic and substituted or unsubstituted, and each aryl and heteroaryl moiety may be substituted or unsubstituted;

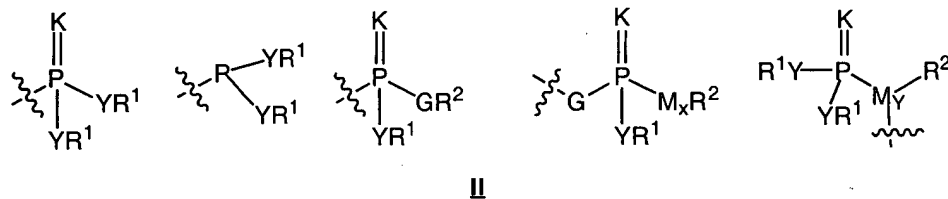
with the following provisos:

(A) (1) R^D is a moiety other than one comprising a substituted or unsubstituted arylene moiety (in which up to two methine carbons may be replaced by nitrogen atoms), a C3-7 cycloalkylene moiety (which may contain nitrogen atoms in place of up to two ring carbons), an indanylene moiety, or a 1,2,3,4-tetrahydronaphthylene moiety; or (2) R^D is a moiety other than one terminating in a cyano group or in an N-substituted or unsubstituted amino, amidino, guanidino or guanidinoalkyl group;

(B) in compounds in which R^C is H, OH, halogen, alkoxy or cycloalkoxy groups of 1 to 6 carbon atoms (which alkoxy and cycloalkoxy groups can be substituted with phenyl) or amine, which can be substituted with phenyl or with alkyl or cycloalkyl groups of 1 to 6 carbon atoms, and R^A is benzyl, phenyl or C1-4 alkyl, optionally substituted with oxygen (e.g. in the form of an ether or alcohol), R^B is a moiety other than a heteroatom- and halogen-substituted derivative of a 3 to 8 carbon cycloalkyl, a 1 to 10 carbon alkyl, a 6 to 13 carbon aryl, or a 7 to 14 carbon aralkyl moiety in which the heteroatom is selected from N, P, S and O; and.

(C) (1) at least one of R^A , R^C or R^D comprises a phosphorus-containing moiety; (2) R^C is covalently attached through a C-C bond to the carbon atom at ring position 2 of the purine ring system; or (3) R^B comprises a phosphorus-containing moiety other than $-P(O)R^J R^{J'}$ where R^J and $R^{J'}$ are independently OH, alkoxy, arylalkoxy, aryloxy, alkylcarbonyloxy-alkoxy, arylalkylcarbonyloxyalkoxy, $NR^k R^{k'}$, mono- or di-alkylaminocarbonylmethoxy, (di-aryl-alkylaminocarbonylmethoxy, arylamino, a D- or L- amino acid, N-alkyl)piperidine-4yloxy, 2-methylsulfonylethoxy, 1,3 thiazole-2-ylmethoxy, 3-pyridylmethoxy, or 2-((di-alkyl)amino)ethoxy, where R^k is H, alkyl, cycloalkyl, cycloalkylalkyl, or aryl or arylalkyl (1-5 carbon atoms of the aryl ring may be replaced with N, O or S), or R^k and $R^{k'}$ together with the atoms that connect them form a ring system (which can also contain additional N, O or S atoms and which can be saturated or unsaturated).

2. The compound of claim 1, wherein the phosphorus-containing moiety in R^B is an aliphatic, heteroaliphatic, aryl, or heteroaryl group which comprises at least one of the substituents set forth in Series II:



wherein each occurrence of K is independently -O- or -S-;

each occurrence of Y is independently -O-, -S-, -NR- or a chemical bond linking R^1 to P;

each occurrence of R (without a further alphanumeric superscript) is independently hydrogen, or a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

each occurrence of R^1 is independently a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or, except in YR^1 moieties in which Y is a covalent bond, R^1 may also be H;

each occurrence of R^2 is independently R^1 , $-PK(YR^1)(YR^1)$, $-SO_2(YR^1)$ or $-C(O)(YR^1)$;

each occurrence of G is independently -O-, -S-, -NR- or M_x ;

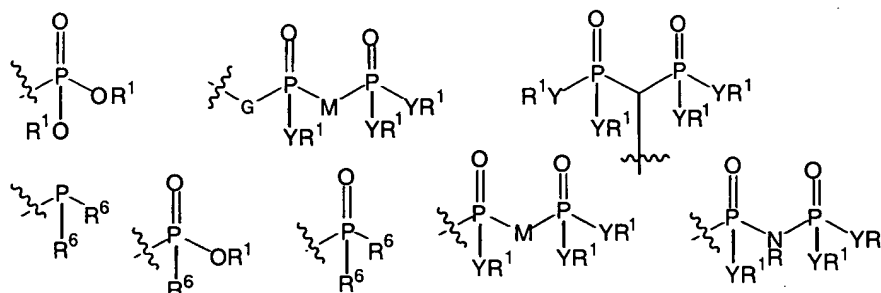
each occurrence of M is independently a substituted or unsubstituted methylene moiety, and any M-M' moiety may be electronically saturated or unsaturated;

each occurrence of x is independently an integer from 1 - 6; and,

each occurrence of My is independently a methine group or a lower alkyl moiety which contains a methine group and optionally may be further substituted.

5

3. The compound of claim 2, wherein the phosphorus-containing moiety in R^B is an aliphatic, heteroaliphatic, aryl, or heteroaryl group which comprises at least one of the substituents set forth in Series IIa:



IIa

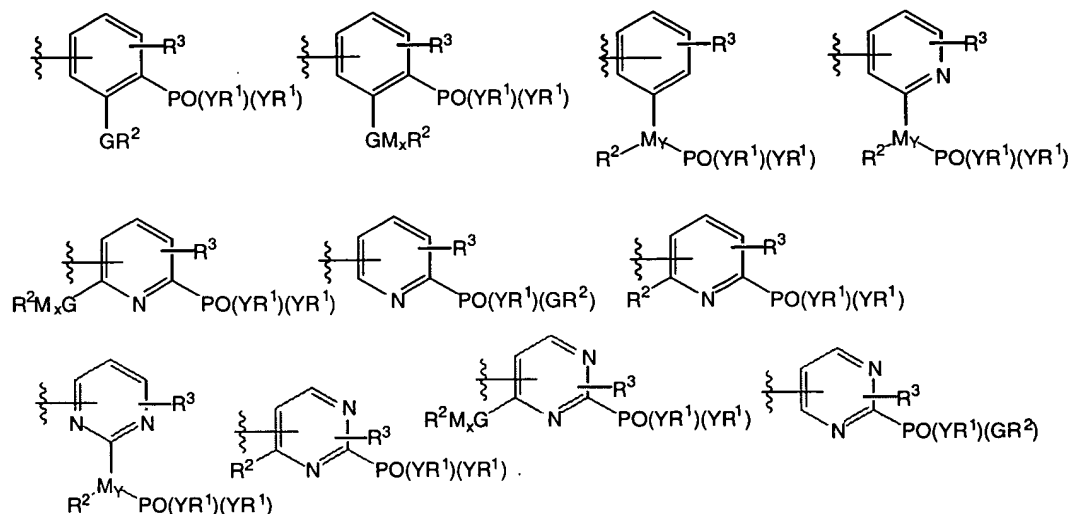
wherein each occurrence of R^6 is an independently selected aliphatic, heteroaliphatic, aryl, or heteroaryl moiety.

15

4. The compound of claim 3 in which R^1 is H or lower alkyl; M is $-\text{CH}_2-$, $-\text{CH}(\text{OH})-$, $-\text{CH}(\text{halo})-$, or $-\text{C}(\text{halo})_2-$; R^6 is lower alkyl and R is H.

5. The compound of claim 1, wherein R^B is any of the aryl or heteroaryl moieties of Series III:

20



III

wherein each occurrence of Y is independently a covalent bond, -O-, -S- or -NR-;

5 each occurrence of R (without a further alphanumeric superscript) is independently hydrogen, or a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

each occurrence of R^1 is independently a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or, except in YR^1 moieties in which Y is a covalent bond, R^1 may also be H;

10 each occurrence of R^2 is independently R^1 , $-PO(YR^1)(YR^1)$, $-SO_2(YR^1)$ or $-C(O)(YR^1)$

each occurrence of R^3 independently represents from 0-3 substituents independently selected from the group consisting of halogen; R, -GR, -CO(YR), acylamino, amido, amidino, cyano, nitro, azido, sulfonyl, sulfoxido, sulfate, sulfonate, sulfamoyl, sulfonamido, and substituents of Series II;

15 each occurrence of G is independently -O-, -S-, -NR- or M_X ;

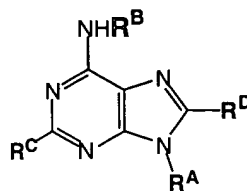
each occurrence of M is independently a substituted or unsubstituted methylene moiety, and any M-M' moiety may be electronically saturated or unsaturated;

20 each occurrence of x is independently an integer from 1 - 6; and,

each occurrence of M_Y is independently a methine group or a lower alkyl moiety which contains a methine group and optionally may be further substituted.

25

6. The compound of formula (I) (or a pharmaceutically acceptable derivative thereof):

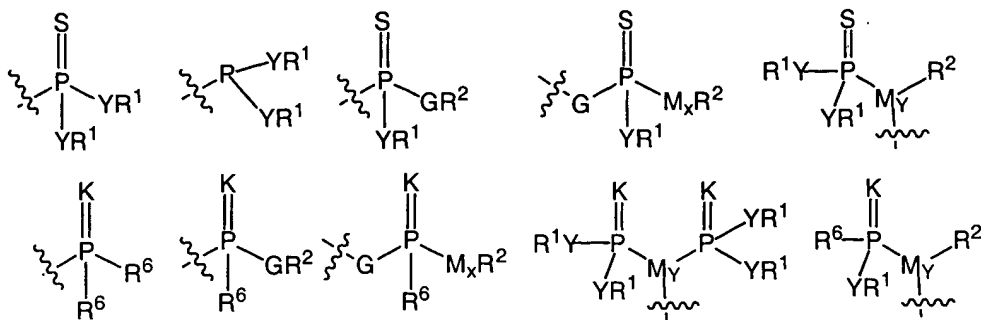


(I)

wherein

R^A is hydrogen, or an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

R^B comprises an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety bearing at least one a substituent of Series IIb:



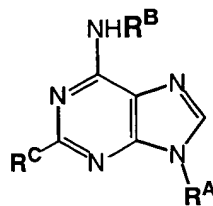
IIb

- 5 R^C is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or -ZR, wherein Z is -O-, -S-, or NR, wherein each occurrence of R without a further alphanumeric superscript is independently hydrogen, or a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

- 10 R^D is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or -ZR; wherein in each of the foregoing groups each aliphatic or heteroaliphatic moiety may be branched or unbranched, cyclic or acyclic and substituted or unsubstituted, and each aryl and heteroaryl moiety may be substituted or unsubstituted;

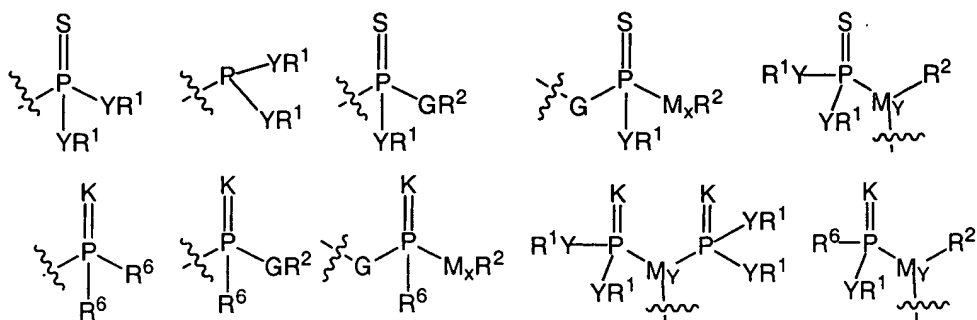
- 15 with the proviso that (1) R^D is a moiety other than one comprising a substituted or unsubstituted arylene moiety (in which up to two methine carbons may be replaced by nitrogen atoms), a C3-7 cycloalkylene moiety (which may contain nitrogen atoms in place of up to two ring carbons), an indanylene moiety, or a 1,2,3,4-tetrahydronaphthylene moiety; or (2) R^D is a moiety other than one terminating in a cyano group or in an N-substituted or unsubstituted amino, amidino, guanidino or guanidinoalkyl group.

- 20 7. The compound of formula (Ia) (or a pharmaceutically acceptable derivative thereof):



(Ia)

- 25 wherein R^A is hydrogen, or an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety; R^B comprises an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety bearing at least one a substituent of Series IIb:

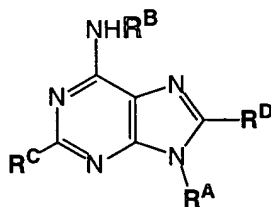


IIb

- R^C is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or -ZR,
 5 wherein Z is -O-, -S-, or NR, wherein each occurrence of R without a further alphanumeric superscript is independently hydrogen, or a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety; and,

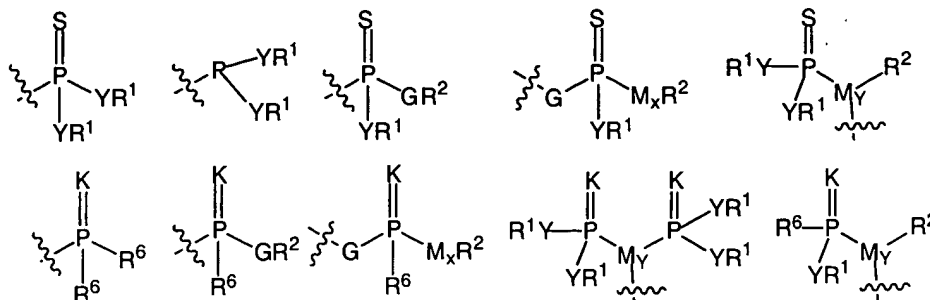
- R^D is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or -ZR;
 wherein in each of the foregoing groups each aliphatic or heteroaliphatic moiety may be
 10 branched or unbranched, cyclic or acyclic and substituted or unsubstituted, and each aryl and heteroaryl moiety may be substituted or unsubstituted.

8. The compound of formula (I) (or a pharmaceutically acceptable derivative thereof):
 15



(I)

- wherein
 R^A is hydrogen, or an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;
 20 R^B comprises an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety bearing at least one a substituent of Series IIb:



IIb

- 5 R^C is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or -ZR, wherein Z is -O-, -S-, or NR, wherein each occurrence of R without a further alphanumeric superscript is independently hydrogen, or a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

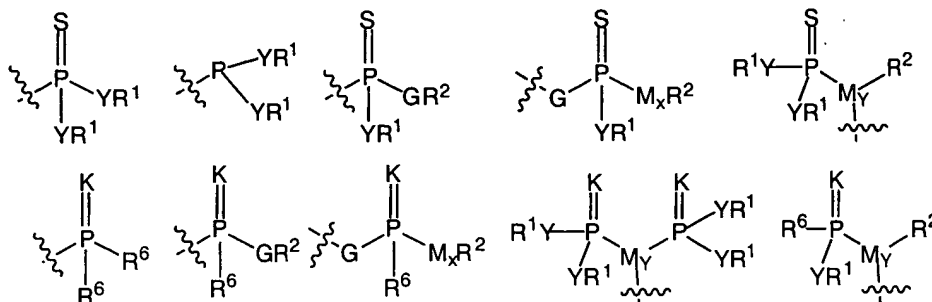
- 10 R^D is hydrogen, halogen, or -YR, wherein R is a moiety which does not terminate in a cyano group or in an N-substituted or unsubstituted amino, amidino, guanidino or guanidinoalkyl group; wherein in each of the foregoing groups each aliphatic or heteroaliphatic moiety may be branched or unbranched, cyclic or acyclic and substituted or unsubstituted, and each aryl and heteroaryl moiety may be substituted or unsubstituted except as provided to the contrary.

- 15 9. The compound of formula (Ia) (or a pharmaceutically acceptable derivative thereof):



(Ia)

- 20 wherein R^A is hydrogen, or an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety; R^B comprises an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety bearing at least one a substituent of Series IIb:

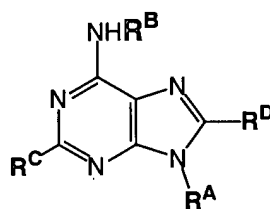


IIb

- 5 R^C is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or -ZR, wherein Z is -O-, -S-, or NR, wherein each occurrence of R without a further alphanumeric superscript is independently hydrogen, or a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

- 10 wherein in each of the foregoing groups each aliphatic or heteroaliphatic moiety may be branched or unbranched, cyclic or acyclic and substituted or unsubstituted, and each aryl and heteroaryl moiety may be substituted or unsubstituted except as provided to the contrary.

10. The compound of formula (I) (or a pharmaceutically acceptable derivative thereof):

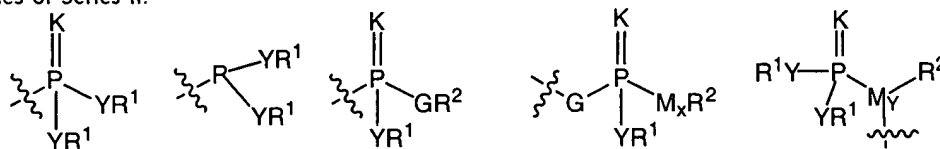


(I)

wherein

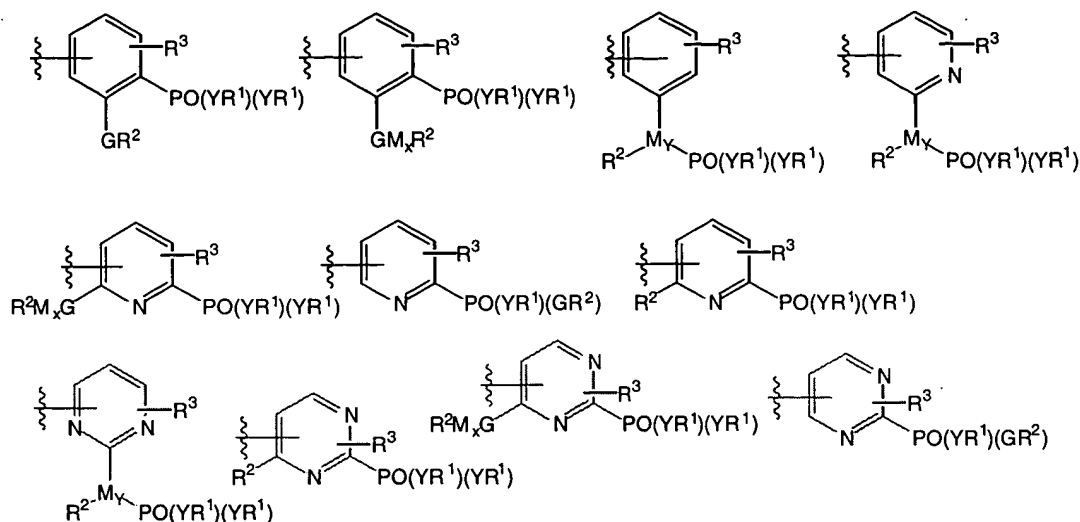
R^A is hydrogen, or an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

R^B is an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety which comprises one or more of the moieties of Series II:



II

or is one of the moieties of Series III:



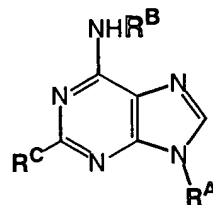
III

R^C is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or -ZR, wherein Z is -O-, -S-, or NR, wherein each occurrence of R without a further alphanumeric superscript is independently hydrogen, or a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

R^D is hydrogen, halogen, or -YR, wherein R is a moiety which does not terminate in a cyano group or in an N-substituted or unsubstituted amino, amidino, guanidino or guanidinoalkyl group; wherein in each of the foregoing groups each aliphatic or heteroaliphatic moiety may be branched or unbranched, cyclic or acyclic and substituted or unsubstituted, and each aryl and heteroaryl moiety may be substituted or unsubstituted;

with the proviso that (1) at least one of R^A , R^C or R^D comprises a phosphorus-containing moiety; (2) R^C is covalently attached through a C-C bond to the carbon atom at ring position 2 of the purine ring system; or (3) R^B comprises a phosphorus-containing moiety other than -P(O)R^JR^{J'} where R^J and R^{J'} are independently OH, alkoxy, arylalkoxy, aryloxy, alkylcarbonyloxy-alkoxy, arylalkylcarbonyloxyalkoxy, NR^kR^{k'}, mono- or di-alkylaminocarbonylmethyloxy, (di-aryl-alkylaminocarbonylmethyloxy, arylamino, a D- or L- amino acid, N-alkyl)piperidine-4yloxy, 2-methylsulfonylethoxy, 1,3 thiazole-2-ylmethyloxy, 3-pyridylmethyloxy, or 2-((di-alkyl)amino)ethoxy, where R^k is H, alkyl, cycloalkyl, cycloalkylalkyl, or aryl or arylalkyl (1-5 carbon atoms of the aryl ring may be replaced with N, O or S), or R^k and R^{k'} together with the atoms that connect them form a ring system (which can also contain additional N, O or S atoms and which can be saturated or unsaturated).

11. The compound of formula (Ia) (or a pharmaceutically acceptable derivative thereof):

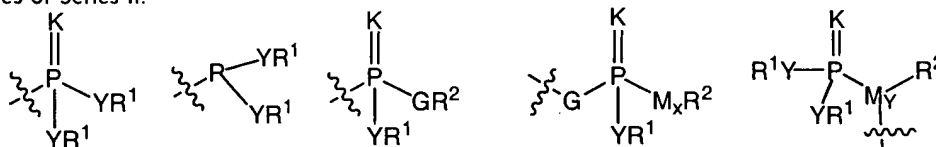


(Ia)

wherein

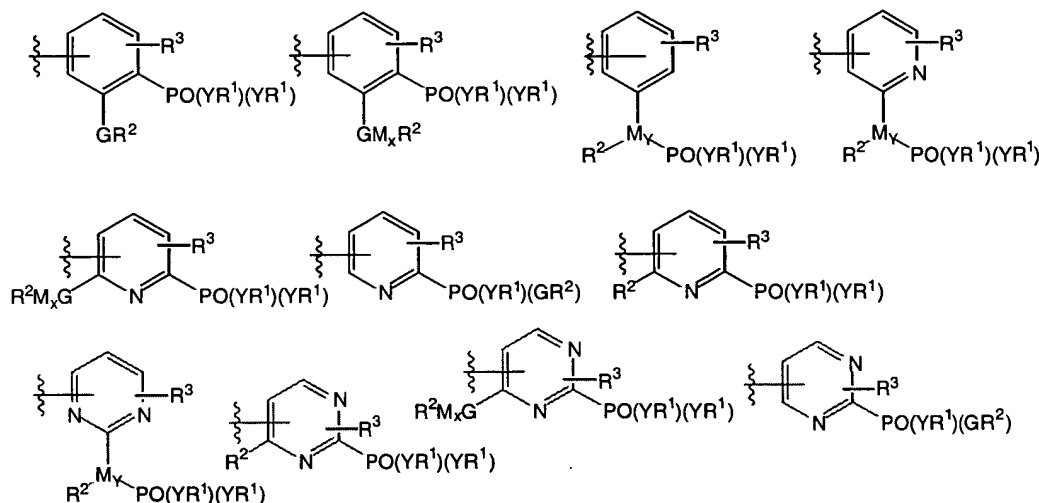
R^A is hydrogen, or an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

- 5 R^B is an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety which comprises one or more of the moieties of Series II:



II

or is one of the moieties of Series III:



III

10

R^C is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or $-ZR$,

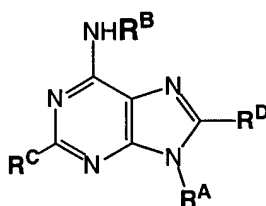
- 15 wherein Z is $-O-$, $-S-$, or NR , wherein each occurrence of R without a further alphanumeric superscript is independently hydrogen, or a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety; and,

wherein in each of the foregoing groups each aliphatic or heteroaliphatic moiety may be branched or unbranched, cyclic or acyclic and substituted or unsubstituted, and each aryl and heteroaryl moiety may be substituted or unsubstituted;

20

with the proviso that (1) at least one of R^A and R^C comprises a phosphorus-containing moiety; (2) R^C is covalently attached through a C-C bond to the carbon atom at ring position 2 of the purine ring system; or (3) R^B comprises a moiety other than $-P(O)R^J R^{J'}$ where R^J and $R^{J'}$ are independently OH, alkoxy, arylalkoxy, aryloxy, alkylcarbonyloxy-alkoxy, arylalkylcarbonyloxyalkoxy, $NR^k R^{k'}$, mono- or di-alkylaminocarbonylmethoxy, (di-aryl-alkylaminocarbonylmethoxy, arylamino, a D- or L- amino acid, N-alkyl)piperidine-4yloxy, 2-methylsulfonylethoxy, 1,3 thiazole-2-ylmethoxy, 3-pyridylmethoxy, or 2-((di-alkyl)amino)ethoxy, where R^k is H, alkyl, cycloalkyl, cycloalkylalkyl, or aryl or arylalkyl (1-5 carbon atoms of the aryl ring may be replaced with N, O or S), or R^k and $R^{k'}$ together with the atoms that connect them form a ring system (which can also contain additional N, O or S atoms and which can be saturated or unsaturated).

12. The compound of formula (I) (or a pharmaceutically acceptable derivative thereof):



(I)

wherein

R^A is hydrogen, or an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

R^B is an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety which comprises one or more phosphorus-containing moieties;

R^C is a branched, unbranched or cyclic alkyl group bearing one or more substituents; a branched, unbranched or cyclic alkoxy moiety substituted with one or more OR, $NR^J R^{J'}$, or substituted aryl moieties; a branched, unbranched or cyclic alkene or alkenoxy moiety which may be optionally substituted with one or more substituents; or $NR^J R^{J'}$ where R and $R^{J'}$ are independently selected from substituted or unsubstituted aliphatic and substituted aryl moieties;

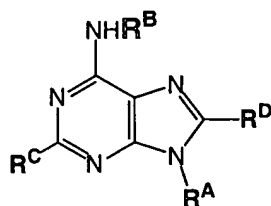
R^D is hydrogen, halogen, or $-YR$, wherein R is a moiety which does not terminate in a cyano group or in an N-substituted or unsubstituted amino, amidino, guanidino or guanidinoalkyl group;

wherein in each of the foregoing groups each aliphatic or heteroaliphatic moiety may be branched or unbranched, cyclic or acyclic and substituted or unsubstituted, and each aryl and heteroaryl moiety may be substituted or unsubstituted;

with the proviso that (1) at least one of R^A , R^C or R^D comprises a phosphorus-containing moiety; (2) R^C is covalently attached through a C-C bond to the carbon atom at ring position 2 of the purine ring system; or (3) R^B comprises a phosphorus-containing moiety other than $-P(O)R^J R^{J'}$ where R^J and $R^{J'}$ are independently OH, alkoxy, arylalkoxy, aryloxy, alkylcarbonyloxy-alkoxy,

arylalkylcarbonyloxyalkoxy, $\text{NR}^k\text{R}^{k'}$, mono- or di-alkylaminocarbonylmethyloxy, (di-aryl-alkylaminocarbonylmethyloxy, arylamino, a D- or L- amino acid, N-alkyl)piperidine-4yloxy, 2-methylsulfonylethoxy, 1,3 thiazole-2-ylmethyloxy, 3-pyridylmethyloxy, or 2-((di-alkyl)amino)ethoxy, where R^k is H, alkyl, cycloalkyl, cycloalkylalkyl, or aryl or arylalkyl (1-5 carbon atoms of the aryl ring may be replaced with N, O or S), or R^k and $\text{R}^{k'}$ together with the atoms that connect them form a ring system (which can also contain additional N, O or S atoms and which can be saturated or unsaturated).

13. The compound of formula (I) (or a pharmaceutically acceptable derivative thereof):



(I)

wherein

R^A is hydrogen; **halogen**; alkenyl; alkynyl; alkyl-; -alkylaryl where the aryl group contains at least one substituent, R^3 ; -alkylheteroaryl which may be optionally substituted; or a substituted aryl or optionally substituted heteroaryl moiety;

R^B is an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety which comprises one or more phosphorus-containing moieties;

R^C is hydrogen; halogen; an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety; or -ZR, wherein Z is -O-, -S-, or NR, wherein each occurrence of R without a further alphanumeric superscript is independently hydrogen, or a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

R^D is hydrogen, halogen, or -YR, wherein R is a moiety which does not terminate in a cyano group or in an N-substituted or unsubstituted amino, amidino, guanidino or guanidinoalkyl group;

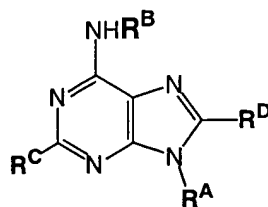
wherein in each of the foregoing groups each aliphatic or heteroaliphatic moiety may be branched or unbranched, cyclic or acyclic and substituted or unsubstituted, and each aryl and heteroaryl moiety may be substituted or unsubstituted;

with the proviso that (1) at least one of R^A , R^C or R^D comprises a phosphorus-containing moiety; (2) R^C is covalently attached through a C-C bond to the carbon atom at ring position 2 of the purine ring system; or (3) R^B comprises a phosphorus-containing moiety other than $-\text{P}(\text{O})\text{R}^J\text{R}^{J'}$ where R^J and $\text{R}^{J'}$ are independently OH, alkoxy, arylalkoxy, aryloxy, alkylcarbonyloxy-alkoxy, arylalkylcarbonyloxyalkoxy, $\text{NR}^k\text{R}^{k'}$, mono- or di-alkylaminocarbonylmethyloxy, (di-aryl-alkylaminocarbonylmethyloxy, arylamino, a D- or L- amino acid, N-alkyl)piperidine-4yloxy, 2-

methanesulfonylethoxy, 1,3 thiazole-2-ylmethoxy, 3-pyridylmethoxy, or 2-((di-alkyl)amino)ethoxy, where R^k is H, alkyl, cycloalkyl, cycloalkylalkyl, or aryl or arylalkyl (1-5 carbon atoms of the aryl ring may be replaced with N, O or S), or R^k and $R^{k'}$ together with the atoms that connect them form a ring system (which can also contain additional N, O or S atoms and which can be saturated or unsaturated).

5

14. The compound of formula (I) (or a pharmaceutically acceptable derivative thereof):



10

wherein

R^A is hydrogen, or an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

R^B is an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety which comprises one or more phosphorus-containing moieties;

15

R^C is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or -ZR, wherein Z is -O-, -S-, or NR, wherein each occurrence of R without a further alphanumeric superscript is independently hydrogen, or a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

20

R^D is hydrogen, halogen, or -YR, wherein R is a moiety which does not terminate in a cyano group or in an N-substituted or unsubstituted amino, amidino, guanidino or guanidinoalkyl group;

at least one of R^A , R^B and R^C also contains an independently selected phosphorus-containing moiety;

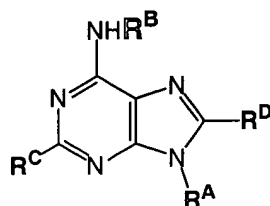
25

wherein in each of the foregoing groups each aliphatic or heteroaliphatic moiety may be branched or unbranched, cyclic or acyclic and substituted or unsubstituted, and each aryl and heteroaryl moiety may be substituted or unsubstituted;

30

with the proviso that in compounds in which R^C is H, OH, halogen, alkoxy or cycloalkoxy groups of 1 to 6 carbon atoms (which alkoxy and cycloalkoxy groups can be substituted with phenyl) or amine, which can be substituted with phenyl or with alkyl or cycloalkyl groups of 1 to 6 carbon atoms, and R^A is benzyl, phenyl or C1-4 alkyl, optionally substituted with oxygen (e.g. in the form of an ether or alcohol), R^B is a moiety other than a heteroatom- and halogen-substituted derivative of a 3 to 8 carbon cycloalkyl, a 1 to 10 carbon alkyl, a 6 to 13 carbon aryl, or a 7 to 14 carbon aralkyl moiety in which the heteroatom is selected from N, P, S and O

15. The compound of formula (I) (or a pharmaceutically acceptable derivative thereof):

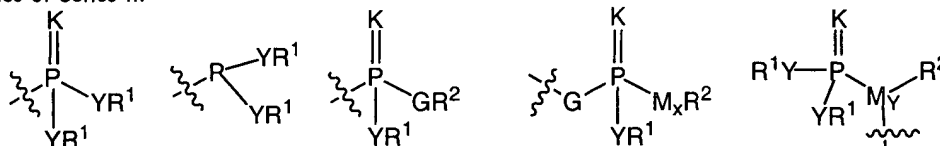


(I)

wherein

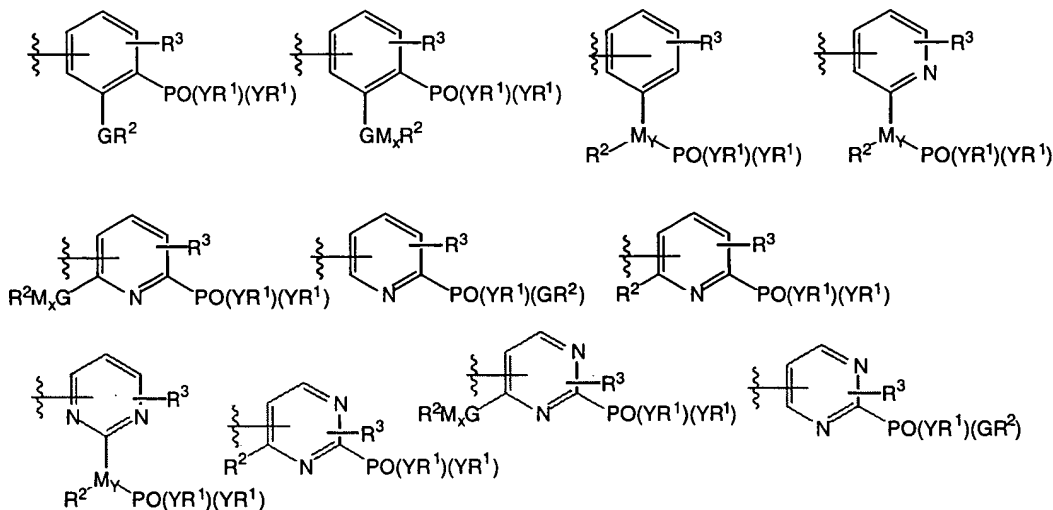
R^A is hydrogen, or an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

R^B is an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety which comprises one or more of the moieties of Series II:



II

or is one of the moieties of Series III:



III

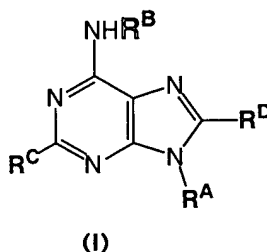
R^C is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or $-ZR$, wherein Z is $-O-$, $-S-$, or NR , wherein each occurrence of R without a further alphanumeric superscript is independently hydrogen, or a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

R^D is hydrogen, halogen, or $-YR$, wherein R is a moiety which does not terminate in a cyano group or in an N -substituted or unsubstituted amino, amidino, guanidino or guanidinoalkyl group;

at least one of R^A , R^B and R^C also contains an independently selected phosphorus-containing moiety;

wherein in each of the foregoing groups each aliphatic or heteroaliphatic moiety may be branched or unbranched, cyclic or acyclic and substituted or unsubstituted, and each aryl and heteroaryl moiety may be substituted or unsubstituted.

16. The compound of formula (I) (or a pharmaceutically acceptable derivative thereof):



wherein

R^A is hydrogen, or an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

R^B is an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety which comprises one or more phosphorus-containing moieties;

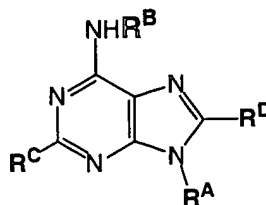
R^C is a branched, unbranched or cyclic alkyl group bearing one or more substituents; a branched, unbranched or cyclic alkoxy moiety substituted with one or more OR, NRR' , or substituted aryl moieties; a branched, unbranched or cyclic alkene or alkenoxy moiety which may be optionally substituted with one or more substituents; or NRR' where R and R' are independently selected from substituted or unsubstituted aliphatic and substituted aryl moieties;

R^D is hydrogen, halogen, or $-YR$, wherein R is a moiety which does not terminate in a cyano group or in an N-substituted or unsubstituted amino, amidino, guanidino or guanidinoalkyl group;

at least one of R^A , R^B and R^C also contains an independently selected phosphorus-containing moiety;

wherein in each of the foregoing groups each aliphatic or heteroaliphatic moiety may be branched or unbranched, cyclic or acyclic and substituted or unsubstituted, and each aryl and heteroaryl moiety may be substituted or unsubstituted.

17. The compound of formula (I) (or a pharmaceutically acceptable derivative thereof):

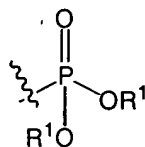


(I)

wherein

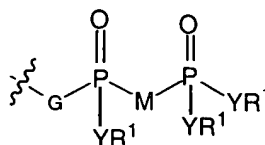
- R^A is hydrogen; **halogen**; alkenyl; alkynyl; alkyl- or alkenyl-aryl where the aryl group contains at least one substituent, R^3 ; or a substituted aryl or heteroaryl moiety; R^B is an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety which comprises one or more phosphorus-containing moieties;
- R^C is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or $-ZR$, wherein Z is $-O-$, $-S-$, or NR , wherein each occurrence of R without a further alphanumeric superscript is independently hydrogen, or a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;
- R^D is hydrogen, halogen, or $-YR$, wherein R is a moiety which does not terminate in a cyano group or in an N-substituted or unsubstituted amino, amidino, guanidino or guanidinoalkyl group;
- at least one of R^A , R^B and R^C also contains an independently selected phosphorus-containing moiety;
- wherein in each of the foregoing groups each aliphatic or heteroaliphatic moiety may be branched or unbranched, cyclic or acyclic and substituted or unsubstituted, and each aryl and heteroaryl moiety may be substituted or unsubstituted;
18. The compound of any of of claims 1 to 17 in which R^D is H or halo.
19. The compound of any of of claims 1 to 18 in which the phosphorus-containing moiety of R^B is present on an aryl or heteroaryl ring system.
20. The compound of any of of claims 1 to 19 in which R^A is lower aliphatic, and may be branched or unbranched, cyclic or acyclic, and optionally substituted with one or more substituents selected from a lower aliphatic group (which may be substituted or unsubstituted), $-OR$, $-SR$, $-NRR'$, $-C(O)YR$, and $-Y-C(O)Y'R$, where Y is O, S, NR, or a bond and R is H or a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety.
21. The compound of claim 20 in which R^A is lower aliphatic which may be substituted with one or more hydroxy, alkoxy, aralkoxy, carbamyl, amino, substituted amino, acyl, cyano, halogen, nitro or sulfo groups, and/or with one or more alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heterocyclic, aryloxy or aralkyl moieties which may themselves be substituted with one or more hydroxy, alkoxy, aralkoxy, carbamyl, amino, substituted amino, acyl, cyano, halogen, nitro or sulfo groups.

22. The compound of claim 20 in which R^A is Mx -aryl or Mx -heterocycle where M is a substituted or unsubstituted methylene, x is an integer from 1 to 6, the aryl moiety may bear one or more substituents, and the heterocycle is a substituted or unsubstituted, aromatic or nonaromatic heterocyclic moiety comprising a 5- to 7-membered ring bearing one or more heteroatoms.
23. The compound of claim 21 wherein M_x is methylene, ethylene or propylene, and the aryl moiety is o-, m-, or p-hydroxy-, 2,3-dihydroxy-, 2,4-dihydroxy-, 2,5-dihydroxy-, 3,4-dihydroxy-, or 3,5-dihydroxyphenyl.
24. The compound of any of claims 1 to 23, wherein R^C is -OR, where R is H, aliphatic, heteroaliphatic, aryl, or heteroaryl.
25. The compound of any of claims 1 to 23, wherein R^C is -R, -NR or -OR in which R is C1-C8 aliphatic, which may be branched or unbranched, cyclic or noncyclic, and which may be substituted with one or more hydroxy, alkoxy, aralkoxy, carbamyl, amino, substituted amino, acyl, cyano, halogen, nitro or sulfo groups, and/or with one or more alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heterocyclic, aryloxy or aralkyl moieties which may themselves be substituted with one or more hydroxy, alkoxy, aralkoxy, carbamyl, amino, substituted amino, acyl, cyano, halogen, nitro or sulfo groups.
26. The compound of any of claims 1 to 23, wherein R comprises a C1-C8 aliphatic moiety substituted with one or more groups selected from the following: a substituted or unsubstituted amine or 5- to 7-membered heterocyclic moiety, which may itself be optionally substituted.
27. The compound of any of claims 1 to 26 in which R^B comprises



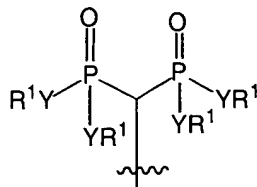
wherein each R^1 is independently H, alkyl, arylalkyl, aryl or a prodrug moiety.

28. The compound of any of claims 1 to 26 in which R^B comprises



wherein each R^1 is independently H, alkyl, arylalkyl, aryl or a prodrug moiety.

29. The compound of any of claims 1 to 26 in which R^B comprises

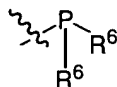


5

wherein each R¹ is independently H, alkyl, arylalkyl, aryl or a prodrug moiety.

30. The compound of any of claims 1 to 26 in which R^B comprises

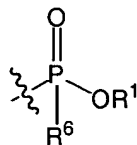
10



wherein each R⁶ is independently alkyl, arylalkyl, aryl or a prodrug moiety.

31. The compound of any of claims 1 to 26 in which R^B comprises

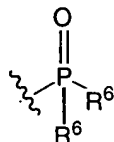
15



wherein R¹ is H, alkyl, arylalkyl or a prodrug moiety and R⁶ is aliphatic, heteroaliphatic, aryl, or heteroaryl or a prodrug moiety.

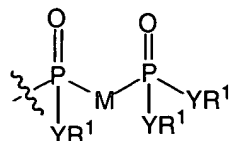
20

32. The compound of any of claims 1 to 26 in which R^B comprises



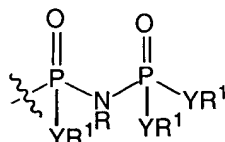
25 wherein each R⁶ is independently aliphatic, heteroaliphatic, aryl, or heteroaryl or a prodrug moiety.

33. The compound of any of claims 1 to 26 in which R^B comprises



wherein each R¹ is H, alkyl, arylalkyl or a prodrug moiety, and Y and M are as defined previously.

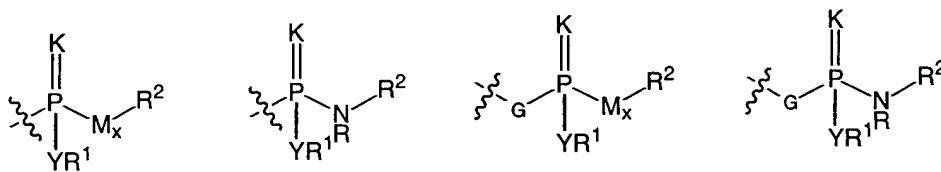
- 5 34. The compound of any of claims 1 to 26 in which R^B comprises



wherein each R¹ is independently H, alkyl, arylalkyl, aryl or a prodrug moiety and R is aliphatic, heteroaliphatic, aryl, or heteroaryl.

10

35. The compound of any of claims 3, 6, 7, 8 or 9 in which R^B comprises one of the following structures



15

in place of a substituent of Series IIa or IIb,

wherein each occurrence of each of the following is as indicated:

G is O, S, NR or M_x;

K is O or S;

- 20 Y is O, S, NR or a chemical bond linking R¹ to P;

R¹ is H, alkyl, arylalkyl or a prodrug moiety;

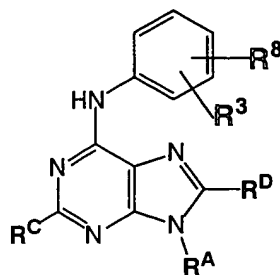
M is substituted or unsubstituted methylene;

x is an integer from 1 to 6; and,

R² is R¹, PK(YR¹)(YR¹), -SO₂(YR¹) or -C(O)(YR¹).

25

36. A compound of formula (Ib) (or a pharmaceutically acceptable derivative thereof):



(1b)

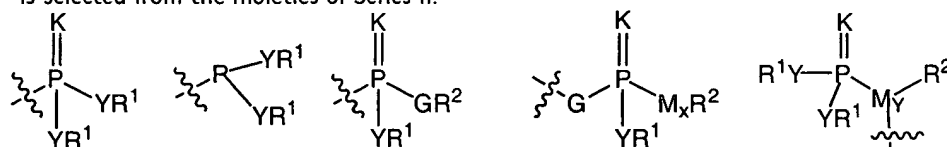
wherein

R^A is hydrogen, or an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

- 5 R^C is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or $-ZR$,
 wherein Z is $-O-$, $-S-$, or NR , wherein each occurrence of R without a further alphanumeric superscript is
 independently hydrogen, or a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl
 moiety;

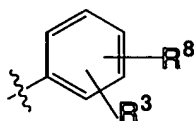
R^D is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or $-ZR$;

- 10 R^8 is selected from the moieties of Series II:



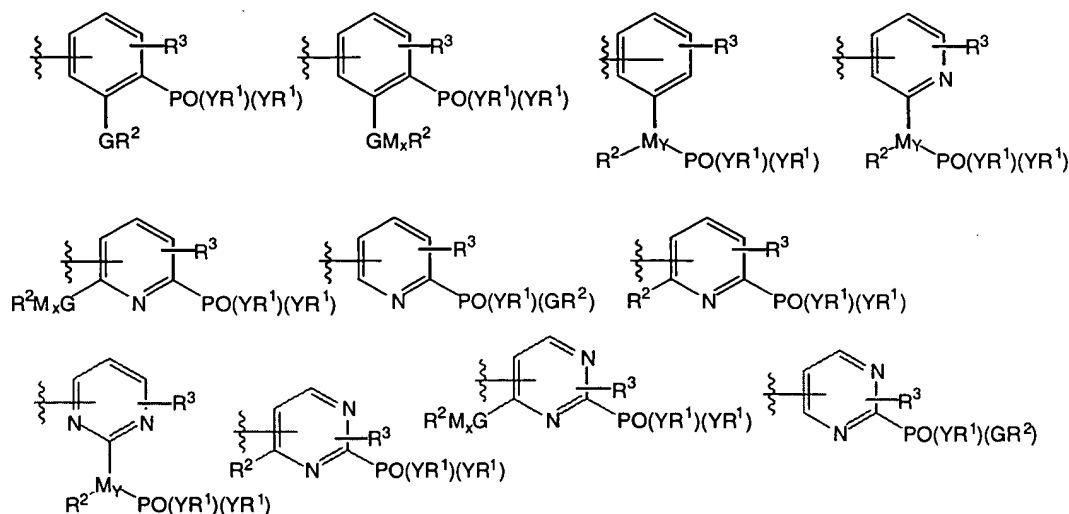
II

or



- 15

is selected from the moieties of Series III:



III

R^3 represents from 0-3 substituents independently selected from the group consisting of halogen; R, -GR, -CO(YR), acylamino, amido, amidino, cyano, nitro, azido, sulfonyl, sulfoxido, sulfate, sulfonate, sulfamoyl, sulfonamido, and substituents of Series II;

5

wherein in each of the foregoing groups each aliphatic or heteroaliphatic moiety may be branched or unbranched, cyclic or acyclic and substituted or unsubstituted, and each aryl and heteroaryl moiety may be substituted or unsubstituted;

with the following provisos:

10

(A) (1) R^D is a moiety other than one comprising a substituted or unsubstituted arylene moiety (in which up to two methine carbons may be replaced by nitrogen atoms), a C3-7 cycloalkylene moiety (which may contain nitrogen atoms in place of up to two ring carbons), an indanylene moiety, or a 1,2,3,4-tetrahydronaphthylene moiety; or (2) R^D is a moiety other than one terminating in a cyano group or in an N-substituted or unsubstituted amino, amidino, guanidino or guanidinoalkyl group;

15

(B) in compounds in which R^C is H, OH, halogen, alkoxy or cycloalkoxy groups of 1 to 6 carbon atoms (which alkoxy and cycloalkoxy groups can be substituted with phenyl) or amine, which can be substituted with phenyl or with alkyl or cycloalkyl groups of 1 to 6 carbon atoms, and R^A is benzyl, phenyl or C1-4 alkyl, optionally substituted with oxygen (e.g. in the form of an ether or alcohol), R^B is a moiety other than a heteroatom- and halogen-substituted derivative of a 3 to 8 carbon cycloalkyl, a 1 to 10 carbon alkyl, a 6 to 13 carbon aryl, or a 7 to 14 carbon aralkyl moiety in which the heteroatom is selected from N, P, S and O; and,

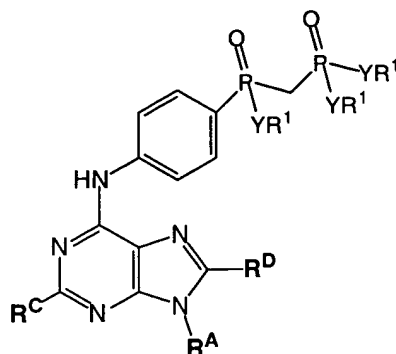
20

(C) (1) at least one of R^A , R^C or R^D comprises a phosphorus-containing moiety; (2) R^C is covalently attached through a C-C bond to the carbon atom at ring position 2 of the purine ring system; or (3) R^B comprises a phosphorus-containing moiety other than $-P(O)R^JR^J'$ where R^J and R^J' are independently OH, alkoxy, arylalkoxy, aryloxy, alkylcarbonyloxy-alkoxy, arylalkylcarbonyloxyalkoxy, $NR^kR^{k'}$, mono- or di-alkylaminocarbonylmethyloxy, (di-aryl-alkylaminocarbonylmethyloxy, arylamino, a D- or L- amino acid, N-alkyl)piperidine-4yloxy, 2-methylsulfonylethoxy, 1,3 thiazole-2-ylmethyloxy, 3-pyridylmethyloxy, or 2-((di-alkyl)amino)ethoxy, where R^k is H, alkyl, cycloalkyl, cycloalkylalkyl, or aryl or arylalkyl (1-5 carbon atoms of the aryl ring may be replaced with N, O or S), or R^k and $R^{k'}$ together with the atoms that connect them form a ring system (which can also contain additional N, O or S atoms and which can be saturated or unsaturated).

30

35

37. The compound (or a pharmaceutically acceptable derivative thereof) of the formula :



wherein

R^A is hydrogen, or an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

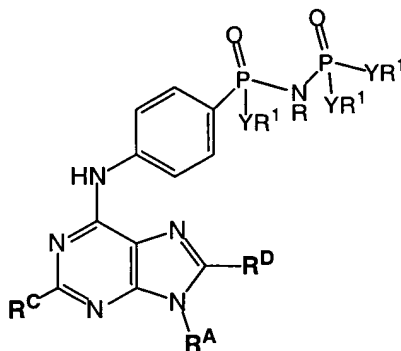
5 R^C is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or -ZR, wherein Z is -O-, -S-, or NR, wherein each occurrence of R without a further alphanumeric superscript is independently hydrogen, or a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

10 R^D is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or -ZR, with the proviso that R^D does not terminate in a cyano group or in an N-substituted or unsubstituted amino, amidino, guanidino or guanidinoalkyl group; and

wherein in each of the foregoing groups each aliphatic or heteroaliphatic moiety may be branched or unbranched, cyclic or acyclic and substituted or unsubstituted, and each aryl and heteroaryl moiety may be substituted or unsubstituted.

15

38. The compound (or a pharmaceutically acceptable derivative thereof) of the formula :



(I)

20

wherein

R^A is hydrogen, or an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

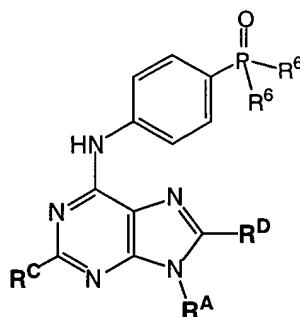
R^C is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or -ZR, wherein Z is -O-, -S-, or NR, wherein each occurrence of R without a further alphanumeric superscript is

independently hydrogen, or a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

- 5 R^D is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or -ZR, with the proviso that R^D does not terminate in a cyano group or in an N-substituted or unsubstituted amino, amidino, guanidino or guanidinoalkyl group; and wherein in each of the foregoing groups each aliphatic or heteroaliphatic moiety may be branched or unbranched, cyclic or acyclic and substituted or unsubstituted, and each aryl and heteroaryl moiety may be substituted or unsubstituted.

10

39. The compound (or a pharmaceutically acceptable derivative thereof) of the formula :



15

wherein

R^A is hydrogen, or an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

R^C is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or -ZR,

wherein Z is -O-, -S-, or NR, wherein each occurrence of R without a further alphanumeric superscript is independently hydrogen, or a substituted or unsubstituted aliphatic, heteroaliphatic, aryl, or heteroaryl moiety;

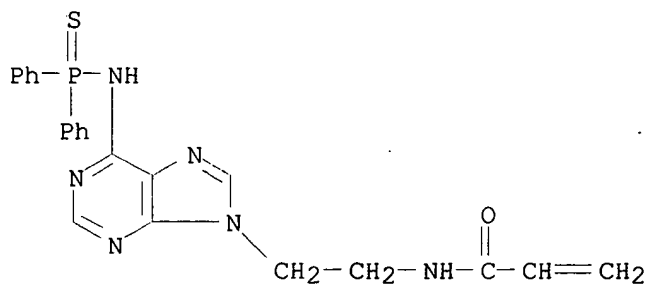
20

- R^D is hydrogen, halogen, an aliphatic, heteroaliphatic, aryl, or heteroaryl moiety, or -ZR, with the proviso that R^D does not terminate in a cyano group or in an N-substituted or unsubstituted amino, amidino, guanidino or guanidinoalkyl group; and wherein in each of the foregoing groups each aliphatic or heteroaliphatic moiety may be branched or unbranched, cyclic or acyclic and substituted or unsubstituted, and each aryl and heteroaryl moiety may be substituted or unsubstituted.

25

40. A composition containing a compound of any of claims 1 to 39 and one or more
30 pharmaceutically acceptable excipient or additive.

41. A pharmaceutical preparation comprising at least one compound of any of claims 1 to 39 or a pharmaceutically acceptable derivative thereof, as inhibitors of bone resorption by osteoclasts, as inhibitors of tumor growth and tumor metastasis, for the treatment and prophylaxis of diseases or undesirable conditions which are mediated by a kinase inhibited by said compound, and at least one pharmaceutically acceptable excipient or additive.
42. A pharmaceutical preparation comprising at least one compound of any of claims 1 to 39 or a pharmaceutically acceptable derivative thereof, and at least one pharmaceutically innocuous excipient or additive.
43. A method for inhibiting bone resorptions, inhibiting tumor growth and/or tumor metastasis, or for the treatment and prevention of diseases or undesirable conditions which are mediated by a kinase inhibited by compound of any of claims 1 to 39, comprising administering a therapeutically effective amount of said compound or a pharmaceutically acceptable derivative thereof to a human or animal in need thereof.
44. A method for inhibiting bone resorption by osteoclasts, comprising administering a therapeutically effective amount of a compound of any of claims 1 to 39, or a pharmaceutically acceptable derivative thereof, to a human or animal in need thereof.
45. A method for inhibiting tumor growth and/or tumor metastasis, comprising administering a therapeutically effective amount of a compound of any of claims 1 to 39, or a pharmaceutically acceptable derivative thereof, to a human or animal in need thereof.
46. A method for the treatment and prophylaxis of diseases which are mediated by a kinase inhibited by a compound of any of claims 1 to 39, comprising administering a therapeutically effective amount of said compound, or a pharmaceutically acceptable derivative thereof, to a human or animal in need thereof.

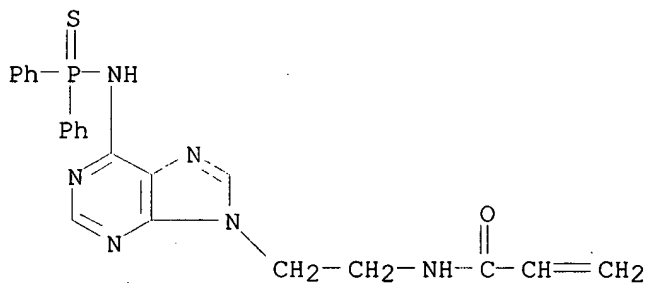


IT 74242-13-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 74242-13-0 HCAPLUS

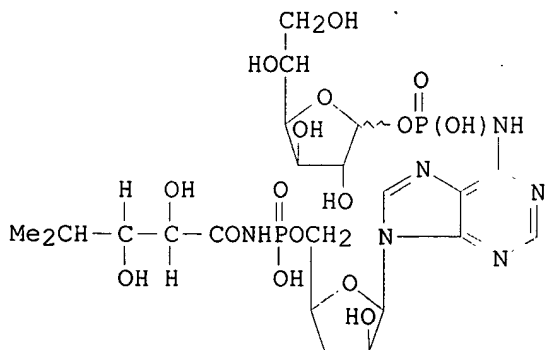
CN 2-Propenamide, N-[2-[6-[(diphenylphosphinothioyl)amino]-9H-purin-9-yl]ethyl]- (9CI) (CA INDEX NAME)



L7 ANSWER 63 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1980:89158 Document No. 92:89158 Adenine N6-substituent of agrocin 84 determines its bacteriocin-like specificity. Tate, M. E.; Murphy, P. J.; Roberts, W. P.; Kerr, A. (Waite Agric. Res. Inst., Univ. Adelaide, Glen Osmond, 5064, Australia). Nature (London), 280(5724), 697-9 (English) 1979. CODEN: NATUAS. ISSN: 0028-0836.

GI



I

AB For the pathogenic strain 57A of Agrobacterium, agrocin 84 (I) [59111-78-3] was 360 times more potent than its nucleotide

Searched by: Mary Hale 308-4258 CM-1 1E01

fragment, nucleoside 5'-phosphoramidate (II) [72666-24-1]. The nonpathogenic strain 57 was not inhibited by agrocin 84 at molarities at which II readily gave inhibition (3.2 .times. 108 agrocin units/mol). These data show that a 5'-phosphoryl link from the fraudulent nucleoside core 9-(3'-deoxy-.beta.-D-threo-pentofuranosyl)adenine to the amide group of D-threo-2,3-dihydroxy-4-methylpentanamide was required for antibiotic activity, but bacteriocin-like specificity was conferred by a D-glucofuranosyloxyphosphoryl substituent at N6 of adenine.

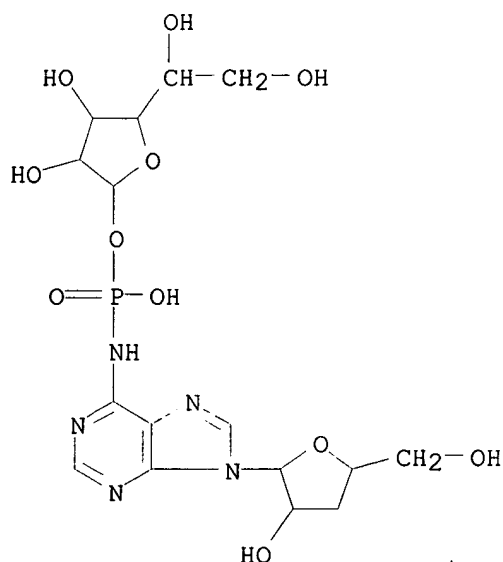
IT **72666-23-0**

RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)

(antibiotic activity of, structure in relation to)

RN 72666-23-0 HCAPLUS

CN D-Glucofuranose, 1-[hydrogen [9-(3-deoxy-.beta.-D-threo-pentofuranosyl)-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)



IT **59111-78-3**

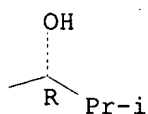
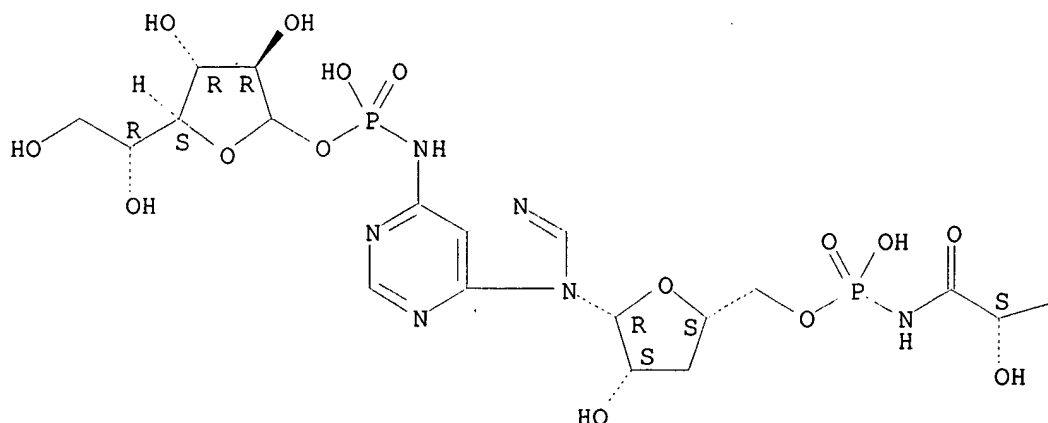
RL: BIOL (Biological study)

(antibiotic and bacteriocin-like specificity of, structure in relation to)

RN 59111-78-3 HCAPLUS

CN D-Glucofuranose, 1-[hydrogen [9-[3-deoxy-5-O-[[[4,5-dideoxy-4-methyl-D-threo-pentonoyl)amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 64 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1980:70165 Document No. 92:70165 A basis for agrocin 84 sensitivity in *Agrobacterium radiobacter*. Murphy, P. J.; Roberts, W. P. (Dep. Agric. Biochem., Waite Agric. Res. Inst., Glen Osmond, 5064, Australia). J. Gen. Microbiol., 114(1), 207-13 (English) 1979. CODEN: JGMIAN. ISSN: 0022-1287.

AB Agrocin 84 (I) [59111-78-3] inhibited a virulent strain of A. *radiobacter* contg. a nopaline Ti plasmid, but not the same strain lacking the Ti plasmid. Sensitivity to I was correlated with its active uptake by a high-affinity transport system with a K_m of $5.88 \times 10^{-8} M$. Unmetabolized I was transported inside the sensitive strain and was assocd. with the sol. fraction of ruptured bacteria and not with the outer walls or cytoplasmic membrane. I bound to a protein fraction isolated from the periplasmic space of the sensitive strain; there was no equiv. binding activity in the insensitive strain. Thus, sensitivity to I may be due to the presence of .gtoreq.1 plasmid-coded binding proteins which are assocd. with I transport into sensitive strains.

IT 59111-78-3

RL: PRP (Properties)

(*Agrobacterium radiobacter* inhibition by, plasmid Ti and transport in relation to)

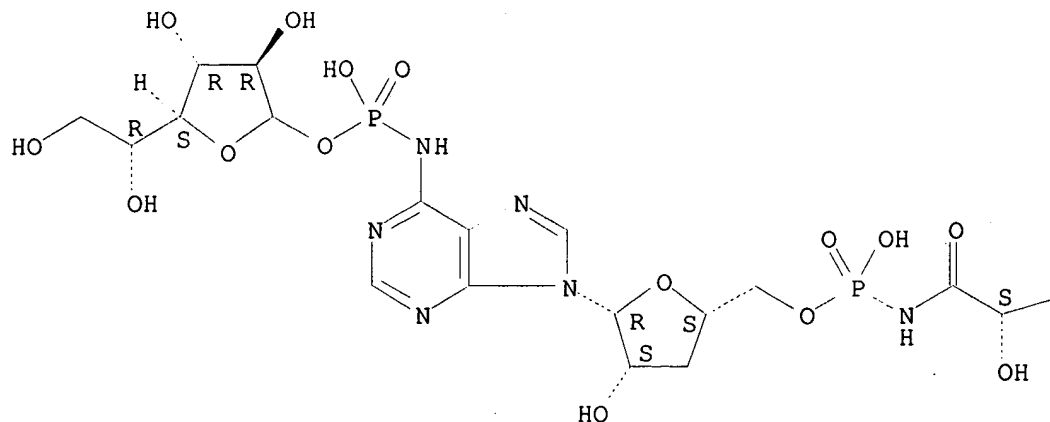
RN 59111-78-3 HCAPLUS

CN D-Glucofuranose, 1-[hydrogen [9-[3-deoxy-5-O-[[[4,5-dideoxy-4-methyl-D-threo-pentonoyl)amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-

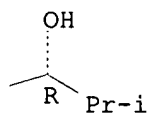
purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



L7 ANSWER 65 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1979:571380 Document No. 91:171380 Purification and characterization of agrocin 84. Thompson, R. J.; Hamilton, R. H.; Pootjes, Christine F. (Dep. Biol., Pennsylvania State Univ., University Park, PA, 16802, USA). Antimicrob. Agents Chemother., 16(3), 293-6 (English) 1979. CODEN: AMACQ. ISSN: 0066-4804.

AB A procedure for the rapid purifn. of milligram quantities of agrocin 84, a bacteriocin-like compd. produced by Agrobacterium radiobacter, was developed. This procedure, which employs charcoal adsorption, ion-exchange and sieving chromatog., and continuous-flow electrophoresis, yielded agrocin 84 which was 65% pure on a dry wt. basis. The purest preps. were strongly UV absorbing, with a max. at 264 nm and a min. at 227 nm. Agrocin 84 contains an unusual phosphoramidate or 6-N-acyl linkage to adenine. Adenine, glucose, and phosphate are present in a 1:1:2 molar ratio. The mol. wt. was estd. to be 1350.

IT 59111-78-3P

RL: PREP (Preparation)

(of Agrobacterium radiobacter, purifn. and characterization of)

RN 59111-78-3 HCAPLUS

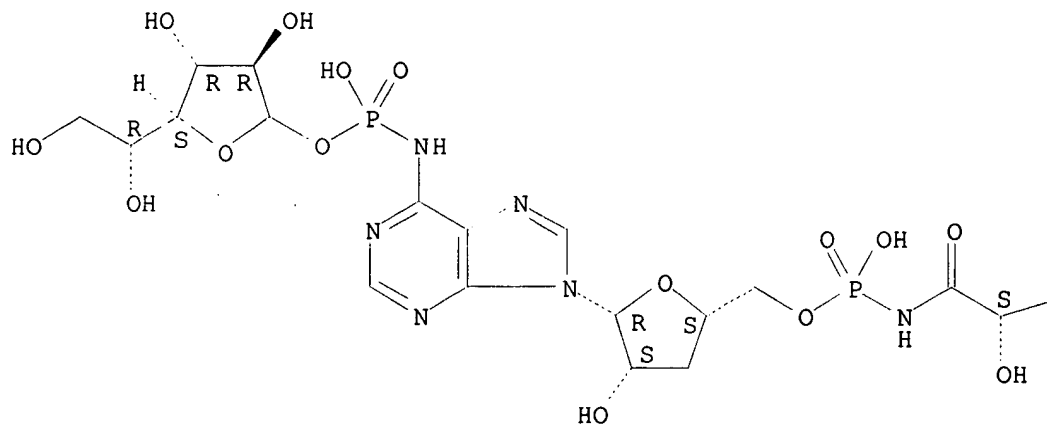
CN D-Glucofuranose, 1-[hydrogen [9-[3-deoxy-5-O-[[[(4,5-dideoxy-4-methyl-D-threo-pentonoyl)amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-

Searched by: Mary Hale 308-4258 CM-1 1E01

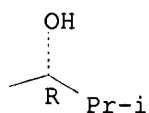
purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



L7 ANSWER 66 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1978:576258 Document No. 89:176258 Interrelationship of pathogenicity, agrocin sensitivity and metabolic characteristics in *Agrobacterium tumefaciens*. Das, P. K.; Basu, M.; Chatterjee, G. C. (Dep. Biochem., Calcutta Univ., Calcutta, India). Sci. Cult., 44(6), 260-5 (English) 1978. CODEN: SCINAL. ISSN: 0036-8156.

AB A review and discussion with 45 refs. concerning the biochem. nature of bacteriocins.

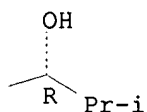
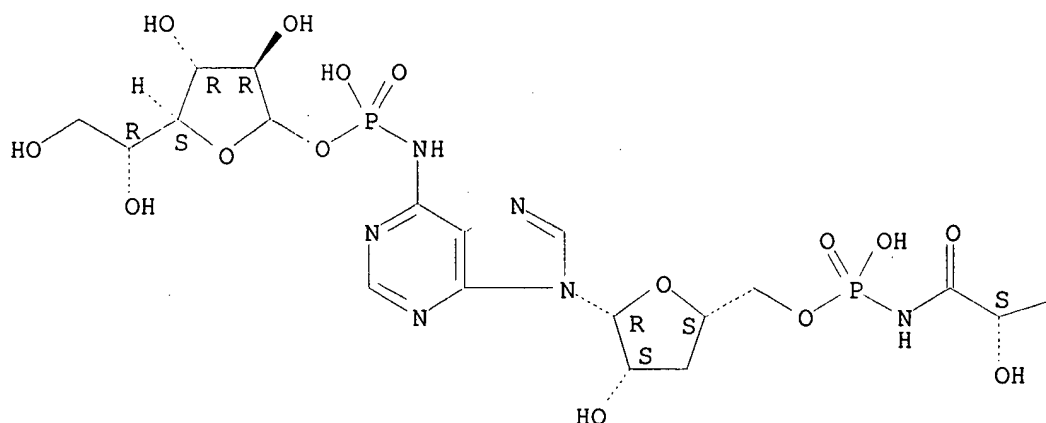
IT 59111-78-3

RL: BIOL (Biological study)
(biochem. nature of)

RN. 59111-78-3 HCAPLUS

CN D-Glucofuranose, 1-[hydrogen [9-[3-deoxy-5-O-[[[(4,5-dideoxy-4-methyl-D-threo-pentonoyl)amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 67 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1978:500793 Document No. 89:100793 Studies on the mode of action of agrocine 84. Das, Pijush K.; Basu, Mitali; Chatterjee, Gora C. (Dep. Biochem., Univ. Calcutta, Calcutta, India). J. Antibiot., 31(5), 490-2 (English) 1978. CODEN: JANTAJ. ISSN: 0021-8820.

AB Agrocine 84 [59111-78-3], a bacteriocin produced by *Agrobacterium radiobacter*, apparently affected sensitive strains of *A. tumefaciens* by inhibiting DNA synthesis. Agrocine 84 did not immediately block DNA formation, however, but was effective only after approx. 30 min of preincubation with the cells. This delayed effect may be due to a transformation of the bacteriocin to an activated form. Agrocine 84 did not possess any DNase activity, did not inhibit RNA or protein synthesis, and did not affect cell permeability.

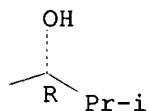
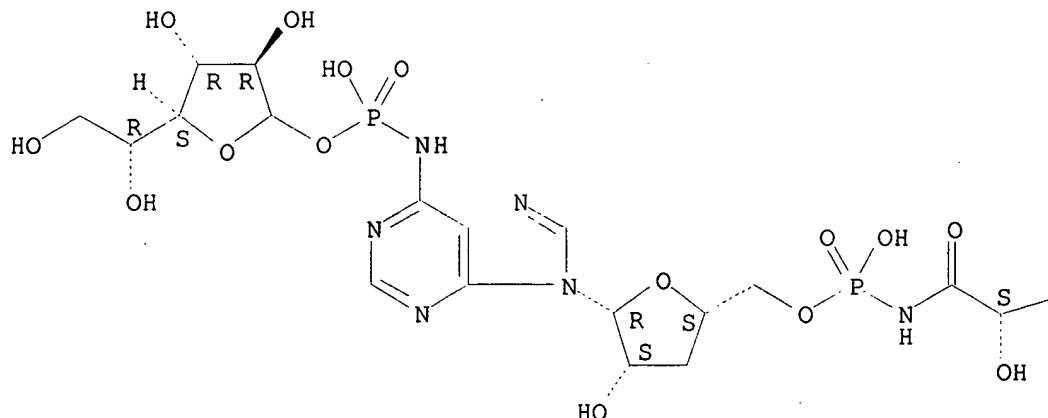
IT 59111-78-3

RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study) (bactericidal action of, DNA formation in relation to)

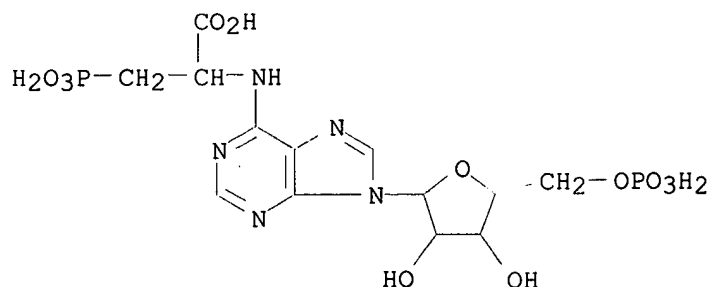
RN 59111-78-3 HCAPLUS

CN D-Glucofuranose, 1-[hydrogen [9-[3-deoxy-5-O-[[[(4,5-dideoxy-4-methyl-D-threo-pentono-yl)amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



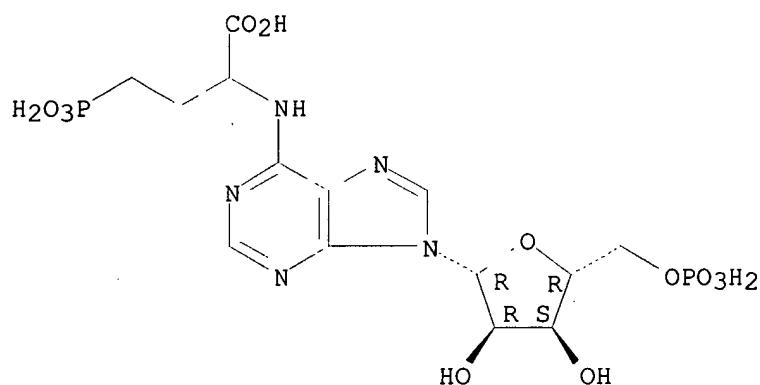
- L7 ANSWER 68 OF 77 HCAPLUS COPYRIGHT 2002 ACS
 1978:438622 Document No. 89:38622 Inhibition of adenylosuccinase by adenylophosphonopropionate and related compounds. Brand, Larry M.; Lowenstein, John M. (Grad. Dep. Biochem., Brandeis Univ., Waltham, Mass., USA). Biochemistry, 17(8), 1365-70 (English) 1978. CODEN: BICHAW. ISSN: 0006-2960.
- AB Adenylosuccinase from muscle, liver, and yeast was strongly inhibited by the substrate analog, adenylophosphonopropionate [N6-(DL-1-carboxy-2-phosphonoethyl)AMP]. The inhibition was freely reversible and of the competitive type, with apparent K_i values of 5.4-86 nM depending on the source of enzyme. Ratios of K_m/K_i with adenylosuccinate as substrate fell in the range 44-1350. Comparison of 4 carboxyl analogs of adenylosuccinate with the corresponding phosphonate analogs showed that the phosphonates were much better inhibitors. Adenylosuccinate analogs in which the .beta.-carboxyl was replaced by other functional groups were much poorer inhibitors. The exceptionally high affinity of adenylosuccinase for adenylophosphonopropionate appears to involve the dianion of the phosphonate group.
- IT 66723-09-9 66723-15-7 66723-16-8
 66723-17-9
 RL: BIOL (Biological study)
 (adenylosuccinase inhibition by, kinetics of)
- RN 66723-09-9 HCAPLUS
- CN Alanine, 3-phosphono-N-[9-(5-O-phosphono-.beta.-D-ribofuranosyl)-9H-purin-6-yl]- (9CI) (CA INDEX NAME)



RN 66723-15-7 HCAPLUS

CN Butanoic acid, 4-phosphono-2-[[9-(5-O-phosphono-.beta.-D-ribofuranosyl)-9H-purin-6-yl]amino]- (9CI) (CA INDEX NAME)

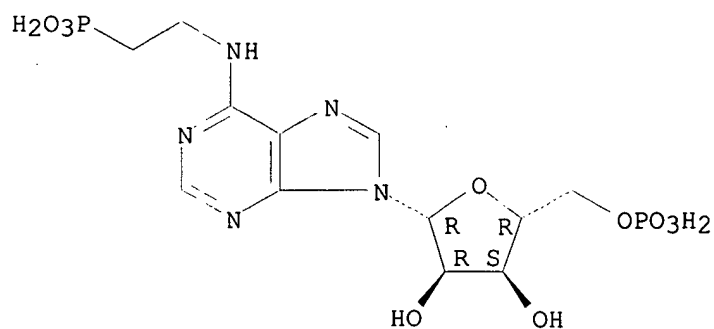
Absolute stereochemistry.



RN 66723-16-8 HCAPLUS

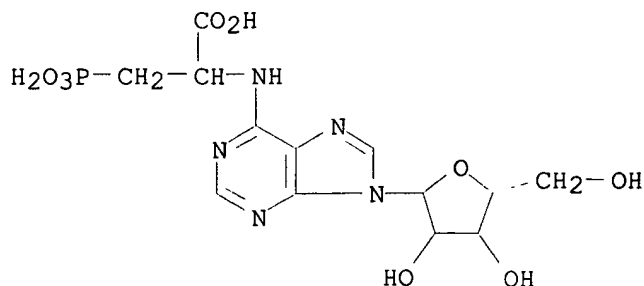
CN 5'-Adenylic acid, N-(2-phosphonoethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

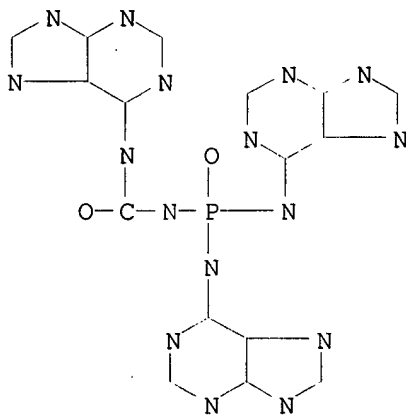


RN 66723-17-9 HCAPLUS

CN Alanine, 3-phosphono-N-(9-.beta.-D-ribofuranosyl-9H-purin-6-yl)- (9CI) (CA INDEX NAME)



L7 ANSWER 69 OF 77 HCAPLUS COPYRIGHT 2002 ACS
 1977:601587 Document No. 87:201587 N-Purinyln-N'-
 [bis(purinylamino)phosphonyl]ureas. Gubnitskaya, E. S.; Cherkasov, V. M.;
 Kurilenko, L. K.; Loseva, I. M.; Derkach, G. I. (Institute of Organic
 Chemistry, Academy of Sciences, Ukrainian S.S.R., USSR). U.S.S.R. SU
 412765 19770705 (Russian). CODEN: URXXAF. APPLICATION: SU 1970-1457304
 19700709.
 AB The title compds. were prepd. by treatment of Cl2P(O)NCO with substituted
 6-aminopurines in the presence of Et3N.
 IT **64196-71-ODP**, derivs.
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 64196-71-0 HCAPLUS
 CN Urea, N-[bis(1H-purin-6-ylamino)phosphinyl]-N'-1H-purin-6-yl- (9CI) (CA
 INDEX NAME)



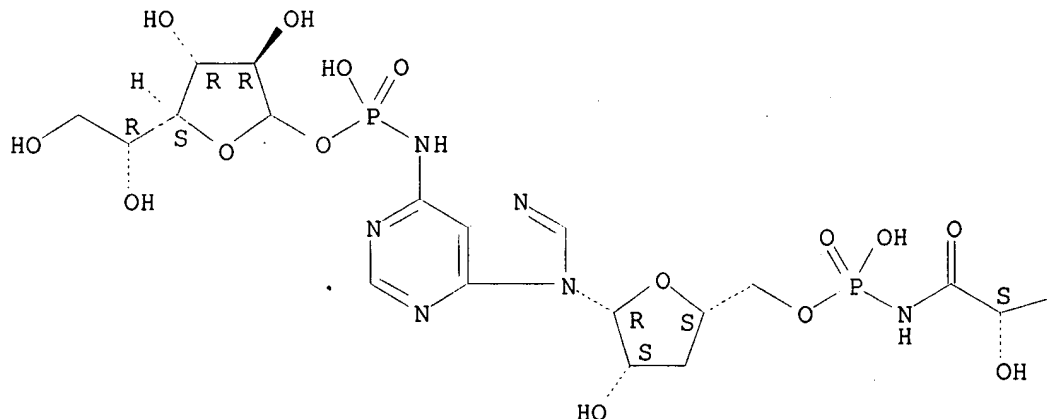
*** FRAGMENT DIAGRAM IS INCOMPLETE ***

L7 ANSWER 70 OF 77 HCAPLUS COPYRIGHT 2002 ACS
 1977:418584 Document No. 87:18584 Agrocine 84 is a 6-N-phosphoramidate of an
 adenine nucleotide analog. Roberts, W. P.; Tate, M. E.; Kerr, A. (Dep.
 Agric. Biochem., Univ. Adelaide, Glen Osmond, Aust.). Nature (London),
 265(5592), 379-81 (English) 1977. CODEN: NATUAS.
 AB Agrocine 84, produced by a rough variant of strain 84 of Agrobacterium
 radiobacter, was purified by gradient elution techniques followed by
 electrophoresis on glass-fiber filter paper, and shown by its IR and UV
 spectra to be a 6-N-phosphoramidate-substituted adenine nucleotide analog.
 IT **59111-78-3**
 RL: PRP (Properties)
 (structure of)

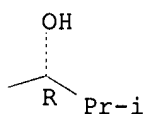
RN 59111-78-3 HCAPLUS
 CN D-Glucofuranose, 1-[hydrogen [9-[3-deoxy-5-O-[[(4,5-dideoxy-4-methyl-D-threo-pentonoyl)amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



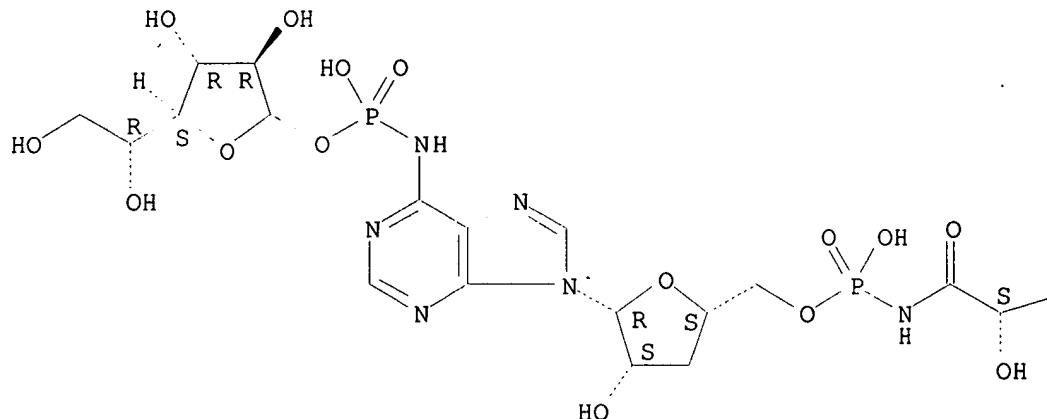
- L7 ANSWER 71 OF 77 HCAPLUS COPYRIGHT 2002 ACS
 1976:554961 Document No. 85:154961 Chemical nature of agrocin 84 and its effect on a virulent strain of *Agrobacterium tumefaciens*. McCardell, Barbara A.; Pootjes, C. F. (Dep. Microbiol., Pennsylvania State Univ., University Park, Pa., USA). *Antimicrob. Agents Chemother.*, 10(3), 498-502 (English) 1976. CODEN: AMACCQ.
- AB Agrocin 84 [59111-78-3], produced by *A. radiobacter* K84, inhibited RNA, DNA, and protein synthesis and amino acid transport in a susceptible, virulent strain of *A. tumefaciens* H-38-9. Cell motility was immediately stopped by action of the agrocin, 50% of the cells were killed within 15 min of contact, and the remainder were inhibited. Agrocin 84 is trypsin and pepsin resistant, but chem. anal. indicated a small peptide with a mol. wt. of 2500 contg. 6 different amino acids, including 9 mols. of glutamine or glutamic acid and 7 mols. of serine.
- IT 59111-78-3
 RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)
 (Agrobacterium tumefaciens response to, compn. in relation to)

RN 59111-78-3 HCAPLUS

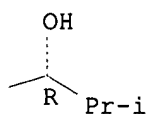
CN D-Glucofuranose, 1-[hydrogen [9-[3-deoxy-5-O-[[[4,5-dideoxy-4-methyl-D-threo-pentonoyl)amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



L7 ANSWER 72 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1976:132392 Document No. 84:132392 Purification of the Agrobacterium radiobacter 84 agrocin. Heip, J.; Chatterjee, G. C.; Vandekerckhove, J.; Van Montagu, M.; Schell, J. (Lab. Genet. Histol., Rijksuniv. Gent, Ghent, Belg.). Arch. Int. Physiol. Biochim., 83(5), 974-6 (English) 1975. CODEN: AIPBAY.

AB The agrocin 84 produced by A. radiobacter 84 was obtained by growing the organism on minimal-agar medium at 27.degree. for 48 hr, freezing the medium at -20.degree., thawing followed by CHCl3 treatment, centrifugation, and pptn. of proteins and nucleic acids by making the soln. 70% in EtOH. The agrocin activity resided in the supernatant, was resistant to pronase, trypsin, RNase, and DNase, and was rather heat stable. The activity was lost upon dialysis, could not be pptd. at 250,000 g for 4 hr, and had a mol. wt. in the range 200-1000 dalton as detd. by gel filtration. Paper electrophoresis indicated it was a highly acidic mol.

IT 59111-78-3

RL: BIOL (Biological study)

Searched by: Mary Hale 308-4258 CM-1 1E01

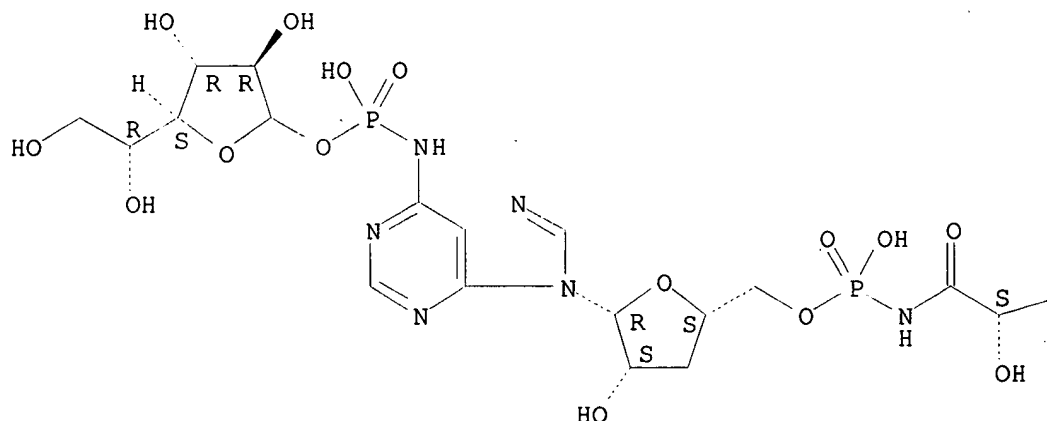
(from Agrobacterium radiobacter)

RN 59111-78-3 HCAPLUS

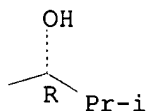
CN D-Glucofuranose, 1-[hydrogen [9-[3-deoxy-5-O-[[(4,5-dideoxy-4-methyl-D-threo-pentonoyl)amino]hydroxyphosphinyl]-.beta.-D-threo-pentofuranosyl]-9H-purin-6-yl]phosphoramidate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



L7 ANSWER 73 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1975:493004 Document No. 83:93004 Stereochemical course of the adenosine triphosphate phosphoribosyltransferase reaction in histidine biosynthesis. Chelsky, Daniel; Parsons, Stanley M. (Dep. Chem., Univ. California, Santa Barbara, Calif., USA). J. Biol. Chem., 250(14), 5669-73 (English) 1975. CODEN: JBCHA3.

AB The product of the 1st reaction in histidine biosynthesis was shown by optical rotation measurements on 3 derivs. to have inverted, .beta. stereochem. at the newly formed bond. This is in contrast to .alpha. linkage expected on the basis of previously obsd. exchange, specificity, and covalent intermediate phenomena. The postulated double displacement mechanism for ATP phosphoribosyltransferase (EC 2.4.2.17) must be modified to account for the product stereochem.

IT 56475-05-9

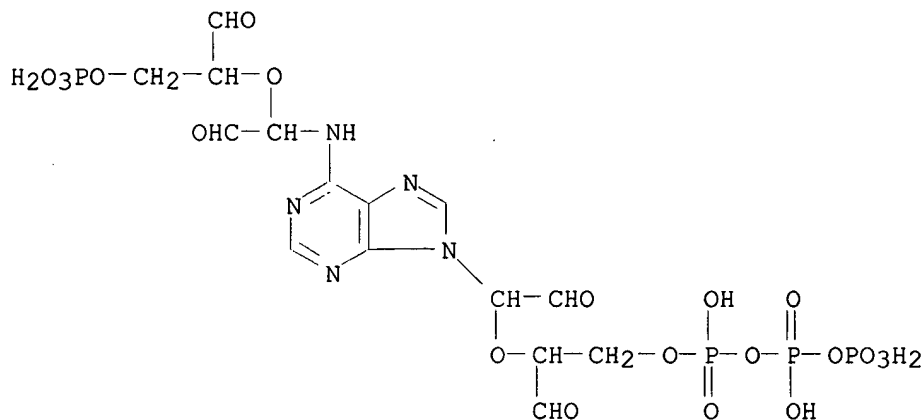
RL: PROC (Process)

(optical rotation of)

RN 56475-05-9 HCAPLUS

Searched by: Mary Hale 308-4258 CM-1 1E01

CN Triphosphoric acid, P-[2-[1-[6-[1-[1-formyl-2-(phosphonooxy)ethoxy]-2-oxoethyl]amino]-9H-purin-9-yl]-2-oxoethoxy]-3-oxopropyl] ester, stereoisomer (9CI) (CA INDEX NAME)



L7 ANSWER 74 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1973:533343 Document No. 79:133343 Mutability of chromosomes of embryonic human cells induced by some analogs of nitrogenous bases. Lekevicius, R.; Kalpokaite, Z.; Jasinskaite, R. (Vil'nyus. Gos. Univ., Vilnius, USSR). Sin. Izuch. Fiziol. Aktiv. Veshchestv, Mater. Konf., 73-4. Vil'nyus. Gos. Univ.: Vilnyus, USSR. (Russian) 1971. CODEN: 26YYAS.

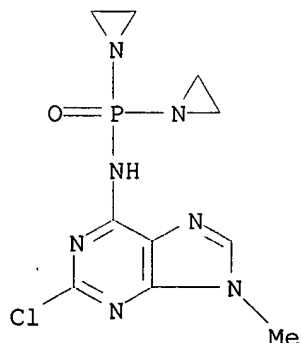
AB Autoradiog. studies with 3T-labeled thymidine showed that 2-chloro-6-diethyleniminophosphamido-9-methylpurine [10154-11-7], 2-chloro-6-bis(.beta.-chloroethyl)aminomethyl-9-methylpurine [13726-50-6], 2-dimethylamino-6-diethyleniminophosphamido-7-methylpurine [42061-52-9], or 2-chloro-6-dimethyleniminophosphamido-7-methylpurine [42061-53-0] increased by 4-6 times the total no. of mutations developing in the chromosomes of 2-month human embryo cells. The proportion of induced mutation types was the same as the proportion obsd. during spontaneous mutagenesis. All 4 compds. increased the length of the mitotic cycle by prolonging the G1 and S stages.

IT 10154-11-7

RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)
(mutagenic activity of, in embryonic cells)

RN 10154-11-7 HCAPLUS

CN Phosphinic amide, P,P-bis(1-aziridinyl)-N-(2-chloro-9-methyl-9H-purin-6-yl)- (7CI, 8CI, 9CI) (CA INDEX NAME)



L7 ANSWER 75 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1972:405431 Document No. 77:5431 Syntheses of purines. XXVI.

6-Bis(ethylenimido)phosphamidopurines. Korsunskii, V. S.; Chaman, E. S.; Golovchinskaya, E. S. (Vses. Nauchno-Issled. Khim.-Farm. Inst. im. Ordzhonikidze, Moscow, USSR). Khim.-Farm. Zh., 6(3), 10-14 (Russian) 1972. CODEN: KHFZAN.

GI For diagram(s), see printed CA Issue.

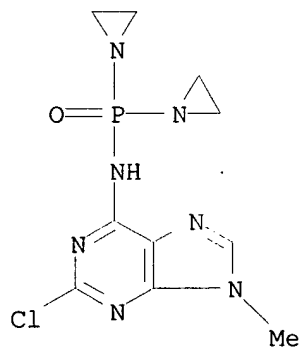
AB ,6-Dichloro-7- and -9-methylpurine reacted with NH₃ to give 2-chloro-7- and -9-methyladenine (I), resp., which gave methyladenines [II and III, resp., R = H, N(CH₂CH:CH₂)₂, piperidino, morpholino; R₁ = H] with III and red P or the corresponding secondary amine. II and III (R₁ = H) were converted to the title compds. [II and III, R₁ = bis(ethylenimido)phosphoro] by treatment with POCl₃ and then ethylenimine. I gave III [R = Cl, R₁ = bis(ethylenimido)phosphoro] with PCl₅ and then HCO₂H. The products had antitumor activity in mice and rats.

IT 10154-11-7P 32600-71-8P 36615-73-3P
36615-74-4P 36615-75-5P 36615-78-8P
36615-79-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

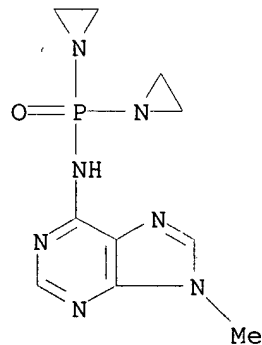
RN 10154-11-7 HCAPLUS

CN Phosphinic amide, P,P-bis(1-aziridinyl)-N-(2-chloro-9-methyl-9H-purin-6-yl)- (7CI, 8CI, 9CI) (CA INDEX NAME)



RN 32600-71-8 HCAPLUS

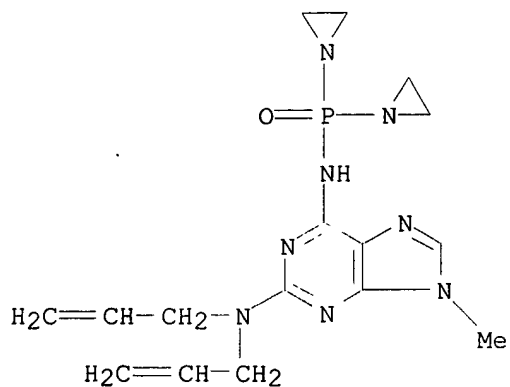
CN Phosphinic amide, P,P-bis(1-aziridinyl)-N-(9-methyl-9H-purin-6-yl)- (8CI, 9CI) (CA INDEX NAME)



RN 36615-73-3 HCAPLUS

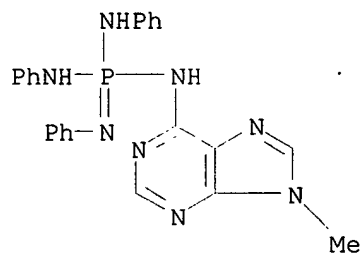
CN Phosphinic amide, P,P-bis(1-aziridinyl)-N-[2-(di-2-propenylamino)-9-methyl-9H-purin-6-yl]- (9CI) (CA INDEX NAME)

Searched by: Mary Hale 308-4258 CM-1 1E01



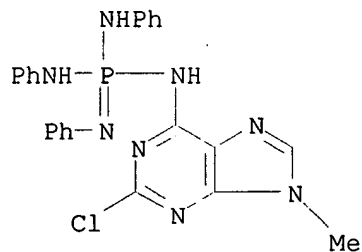
RN 36615-74-4 HCAPLUS

CN Phosphorimidic triamide, N-(9-methyl-9H-purin-6-yl)-N',N'',N'''-triphenyl- (9CI) (CA INDEX NAME)



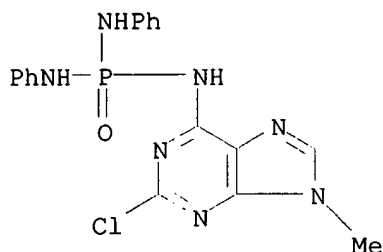
RN 36615-75-5 HCAPLUS

CN Phosphorimidic triamide, N-(2-chloro-9-methyl-9H-purin-6-yl)-N',N'',N'''-triphenyl- (9CI) (CA INDEX NAME)

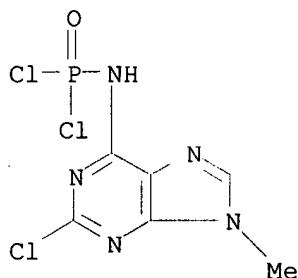


RN 36615-78-8 HCAPLUS

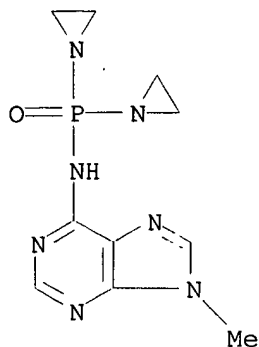
CN Phosphoric triamide, N-(2-chloro-9-methyl-9H-purin-6-yl)-N',N''-diphenyl- (9CI) (CA INDEX NAME)



RN 36615-79-9 HCAPLUS
 CN Phosphoramidic dichloride, (2-chloro-9-methyl-9H-purin-6-yl)- (9CI) (CA INDEX NAME)



L7 ANSWER 76 OF 77 HCAPLUS COPYRIGHT 2002 ACS
 1971:435943 Document No. 75:35943 Diethylenimidophosphamido derivatives of purine. Korsunskii, V. S.; Golovchinskaya, E. S. (Vses. Nauchno-Issled. Khim.-Farm. Inst., Moscow, USSR). Puti Sin. Izyskaniya Protivoopukholevykh Prep., Volume Date 1968, No. 3, 323-9 (Russian) 1970. CODEN: PSIPA4.
 AB Chlorination with Cl of caffeine (I) and isocaffeine (II) gave the 8-trichloromethyl derivs. of I and II. The next Cl atom entered the 7-Me of I or the 3-Me of II. The former deriv. was hydrolyzed to theophylline and the latter to 1,9-dimethylxanthine. 7-Methyl- or 9-methyladenine (III or IV, resp.) was treated with POCl₃ and the resulting dichloride of amidophosphoric acid treated with ethylenimine and HCl acceptors to give both 6-diethylenimidophosphoramido derivs. of III and IV, which were tested against sarcomas 45 and 37, and carcinoma NK. The growth retardations were 60-80, 49-56, and 37-48%, resp. The activity of the III deriv. was slightly higher than that of IV. IV was also prepd. from trihydroxypurine (ureic acid), via 1,9-dimethylxanthine and the 9-Me deriv. of 2,6-dichloropurine (V). Similarly, III was prepd. from theobromine via the 7-Me deriv. of V.
 IT **32600-71-8P**
 RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)
 RN 32600-71-8 HCAPLUS
 CN Phosphinic amide, P,P-bis(1-aziridinyl)-N-(9-methyl-9H-purin-6-yl)- (8CI, 9CI) (CA INDEX NAME)



L7 ANSWER 77 OF 77 HCAPLUS COPYRIGHT 2002 ACS

1967:420237 Document No. 67:20237 Analysis of the cytogenetic and cytostatic effects of 2-chloro-6-(diethyleniminophosphamido)-9-methylpurine on the cells of the Ehrlich carcinoma. Dubinin, N. P.; Lekevicius, R. (Inst. Gen. Genet., Moscow, USSR). Genetika (Moscow) (2), 3-11 (Russian) 1967. CODEN: GNKAA5.

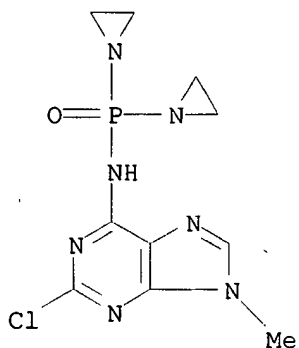
AB A cytogenetic effect of a single dose of 2-chloro-6-(diethyleniminophosphamido)-9-methylpurine applied at $10^{-5}M$ is described. This effect continued through several cell generations both on normal human tissue culture and on Ehrlich ascites tumor cell. The decrease of mitotic activity in subsequent generations was observed in normal cells only. The frequency of chromosomal mutation at this concn. was trebled. Rearrangements of chromosomes do not affect the redn. of mitotic activity.

IT 10154-11-7

RL: BIOL (Biological study)
(neoplasma response to)

RN 10154-11-7 HCAPLUS

CN Phosphinic amide, P,P-bis(1-aziridinyl)-N-(2-chloro-9-methyl-9H-purin-6-yl)- (7CI, 8CI, 9CI) (CA INDEX NAME)



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COST IN U.S. DOLLARS

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

CA SUBSCRIBER PRICE

SINCE FILE	TOTAL
ENTRY	SESSION
296.20	976.06

SINCE FILE	TOTAL
ENTRY	SESSION
-41.51	-117.03

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STN INTERNATIONAL LOGOFF AT 13:33:53 ON 21 JUN 2002

Searched by: Mary Hale 308-4258 CM-1 1E01